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Modeling Crystalline Silicotitanate Performance to Support TCCR Batch 1 and Batch 1A Operations (U)

T. Hang

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EXECUTIVE SUMMARY

The objective of this work is to calculate the expected ion-exchange (IX) column performances of the Tank Closure Cesium Removal (TCCR) system for Tank 10H closure. Savannah River National Laboratory (SRNL) utilized: (1) the ZAM computer program (Version 4) developed by Texas A&M University for prediction of cesium loading on the crystalline silicotitanate (CST) media, (2) the OLI Studio™ software (Version 9.6) from OLI Systems to estimate waste solution properties, and (3) the VERSE-LC code (Version 7.8) developed by Purdue University to calculate column performances.

The study specifically evaluates the TCCR system performance to process Tank 10H Batch 1A supernate.

Results Summary

VERSE-LC was applied to predict TCCR column performances. A parametric study was conducted to evaluate the impact of different parameters (i.e., column configuration, temperature, flow rate, CST particle size) on the column performance. The evaluation indicates:

- TCCR performance is improved at slower process flow rate, at lower operating temperature, and with smaller CST particle size.
- Multi-column configurations are recommended, because the single-column configuration does not utilize the CST bed effectively.
- Use of newer VERSE-LC parameters based on recent Hanford and SRNL CST studies better represent experimental data.

A correction factor (CF), referred to in the past as “dilution factor”, is used in the modeling to offset the difference in performance between the powdered form of CST (which is what the ZAM model is based on) and the engineered media that dilutes the powdered CST with a binder. In addition to the traditionally used value of 0.68, a correction to the binder dilution factors were needed for this tank waste and the combined correction is estimated to be 0.251 based on the Tank 10H teabag tests and 0.464 based on SRNL batch contact tests. The correction factors appear to be lower than traditional binder dilution factors alone due to competing ions or precipitates rather than an increased amount of binder.

VERSE-LC was utilized to predict the TCCR column performance in several operational scenarios in which the impact of the column configurations (i.e., two columns (lead-lag) or three columns (lead-lag-guard) in series), binder correction factors, process flow rates on the column performance was evaluated. The prediction results are summarized in Table E-1. As shown, correction factors of 0.251 and 0.68 provide lower and upper bound performance results, respectively, while correction factor of 0.464 delivers the results close to the TCCR actual performance. The results confirm that the TCCR performance is improved at slower process flow rate. Bucket-average concentration delays the column breakthrough because it is based on a volume-average concentration.

Table E-1. VERSE-LC Results for Batch 1A TCCR Operation at 34 °C

Cases	Column Configuration	Correction Factor η_{CF}	Flow Rate (gpm)	BVs at First DF Breakthough [(a)]
5a	Lead-lag	0.464	5	1352 [1763]
5b	Lead-lag-guard	0.464	3	3169 [3863]
5c	Lead-lag	0.251	5	733 [955]
5d	Lead-lag-guard	0.251	3	1715 [2091]
5e	Lead-lag	0.68	5	1981 [2584]
5f	Lead-lag-guard	0.68	3	4644 [5660]

[(a)]: Based on column effluent concentration; BVs: Bed Volumes; DF: Decontamination Factor of 1000
[]: Based on bucket-average concentration

To better assist Savannah River Remediation (SRR) in future TCCR operations, it is essential to benchmark VERSE-LC predictions against operational/test column data. It is also necessary to further investigate the cause of the much lower binder dilution/correction factors for the teabag and batch contact testing. The results suggest there may be unknown competitor(s) or precipitant(s) that potentially interfere with the adsorption of cesium, which can substantially impact the effectiveness and cost of future use of CST.

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LIST OF ABBREVIATIONS

BVs	Bed Volumes
CF	Binder Correction/Dilution Factor
CST	Crystalline Silicotitanate
DF	Decontamination Factor
gpm	Gallons per Minute
IX	Ion Exchange
SRNL	Savannah River National Laboratory
SRR	Savannah River Remediation
SRS	Savannah River Site
TCCR	Tank Closure Cesium Removal
VDS	Variable Depth Sample

1.0 Introduction

1.1 Background

The TCCR system is a demonstration "at-tank" process designed to remove cesium from aqueous tank waste. Cesium will be removed by ion exchange using engineered IONSIV™ R9120-B[1] form of the CST media.

The TCCR modular enclosure is deployed at Tanks 10 and 11 in the H Tank Farm. Water will be added to the saltcake in Tank 10H to dissolve it. The dissolved salt solution waste will be pumped out of Tank 10H, through pre-filters and ion exchange columns. The decontaminated salt solution will be transferred to nearby Tank 11 (see Figure 1) and on to Tank 50H for final disposal in the Saltstone Production Facility. Cesium will be removed by adsorption onto the CST media. The current TCCR design can accommodate lead-lag (two-column) or lead-lag-guard (three-column) configurations to optimize media utilization and achieve the target decontamination. For example, in a lead-lag configuration, once the target breakthrough (e.g., decontamination factor of 1000) at the lag column outlet is reached, the lead column will be removed from service, the lag column will rotate into the lead position, and a new column will be placed into the lag position. The TCCR process for cesium removal from Tank 10H is detailed in X-SOW-H-00002 (Caldwell, 2017).

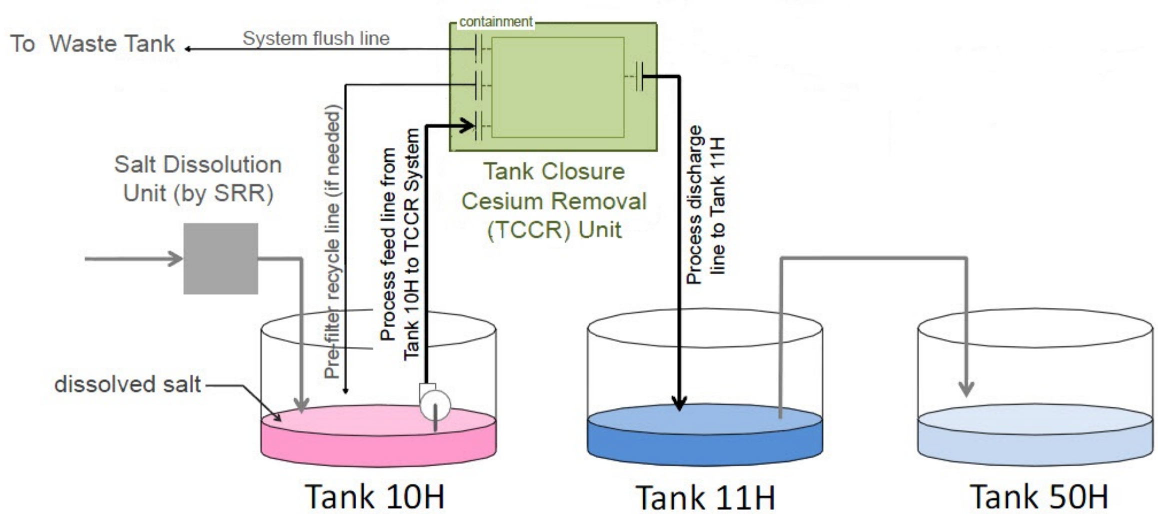

Figure 1. Cesium Removal from Tank 10H

A computer model was developed by the Texas A&M inventors of CST to predict the adsorption of cesium on the media (Zheng et al., 1995; Zheng et al., 1996). That model, known as ZAM, calculates the equilibrium condition for a liquid in contact with the CST. Such equilibrium is dependent upon several factors, including temperature, ionic strength, and concentrations of cesium, potassium, sodium, hydroxide, rubidium, and strontium. For this task, it is important to understand that the CST and the aqueous stream reach an equilibrium condition, not a saturation of the CST. The *total* cesium capacity of CST is much higher than usually encountered in SRS tank waste, but that total capacity cannot be reached because the loading under any condition is thermodynamically limited by the equilibrium, which depends on the composition of the aqueous stream. The ZAM model always calculates the maximum loading of cesium onto CST for the specific temperature and composition, given a specified amount of liquid feed. The

[1] IONSIV is a registered trademark of Honeywell UOP, Des Plaines, IL, U.S.A.

loading is calculated by varying cesium concentrations to generate an isotherm curve across the cesium concentration range for that chemical composition. Conversely, the liquid-to-solid ratio used in the model can be varied to produce an isotherm curve. That isotherm is then translated into an algebraic equation that can be used by the dynamic model (VERSE-LC). The maximum cesium loading depends on temperature, species/composition, and can be calculated based on the feed concentration of cesium so that it is not liquid volume dependent. The model accounts for the temperature, the density, the composition of the aqueous phase, and the two types of exchange sites that exist on the CST solid. The model has been used previously to predict loading on CST for both Savannah River Site (SRS) and Hanford tank waste applications (Aleman and Hamm, 2003; Hamm et al., 2001; Smith 2011).

Because the original CST was in the powdered form of very fine particulates, it was converted to an engineered porous bead form so that it could be used in flow-through columns with moderate pressures. The bead consists of the CST powder and a binder material. The binder material essentially dilutes the CST powder, which would be expected to cause a reduction in cesium adsorption per unit weight of the material. Because the ZAM model was developed for the powdered form of CST, it is expected that there would be an "offset" of the adsorption performance for the engineered bead. To determine the magnitude of this offset, SRNL used the ZAM model and compared it to measured results in prior experimental work with radioactive tank waste samples. It is also worth noting that there are three isotopes of cesium in the SRS tank waste, ^{133}Cs, ^{135}Cs, and ^{137}Cs (Reboul, 2017). The CST removes all isotopes equally. The primary isotope of concern is the ^{137}Cs due to its high specific activity. Although strontium is known to compete with cesium loading, the soluble strontium concentration in Tank 10H waste is insignificant, and therefore its effect is negligible.

To model IX column performance, the dynamic simulation VERSE-LC (VErsatile Reaction SEperation Simulation for Liquid Phase Adsorption and Chromatography Processes) code was chosen based on its availability and widespread (and accepted) use in this field. VERSE-LC, developed by Professor Linda Wang of Purdue University in the 1990s, was written in FORTRAN 90 and available on various platforms (Berninger et al., 1991). SRNL procured an executable file running on the PC/Windows platform.

1.2 Task Objective

SRR requested that SRNL model the TCCR IX process for various TCCR scenarios (Britanisky 2018). Therefore, the task objective is to utilize ZAM for prediction of cesium loading on the TCCR CST media. ZAM calculations are to be compared with data from the in-tank "teabag tests" and SRNL's batch contact tests. VERSE-LC is applied to model IX column performance to aid in the TCCR operations. Column model calculations provide SRR with information on column breakthrough, CST bed utilization, and crucial parameters (e.g., flow rate, temperature, media particle size etc.) that affect the TCCR process.

1.3 Technical Reviews and Quality Assurance

Requirements for performing reviews of technical reports and the extent of review are established in manual E7 2.60. SRNL documents the extent and type of review using the Technical Report Design Checklist (SRNL 2004).

The reviewers of this report include D. J. McCabe, J. L. Wohlwend, and J. A. Dyer. McCabe provides an overall review. Wohlwend reviews the ZAM calculations. Dyer design-checks the VERSE-LC predictions.

2.0 Model Formulations

2.1 Modeling Approach

- The OLI Studio™, a commercial software (Version 9.6) from OLI Systems, Inc. (OLI Systems, 2018), was used to calculate charge balanced feed compositions and to estimate feed solution density, viscosity and diffusivity required as input data to ZAM and VERSE-LC.
- Cesium loading on the CST media in the TCCR ion exchange columns was predicted using a computer program (Version 4) developed by the research group of Professor Rayford G. Anthony of TAMU (Zheng et al., 1997). The ZAM program, named after its developers (i.e., Zheng, Anthony, and Miller), was described in detail in previous ion exchange studies at SRNL (Hamm et al., 2001; Hang et al., 2017).
- CST column performance in the TCCR process was modeled by VERSE-LC (Version 7.8). The VERSE-LC Fortran 90 code was developed by a research group of chemical engineers at Purdue University (Berninger et al., 1991). The code has been utilized in many IX projects at SRS and Hanford (Hamm et al., 2001; Smith 2011).

Note that both ZAM and VERSE effectively handle the temperature condition via the specified properties input data (i.e., temperature, density for ZAM; viscosity, density, diffusivity, and isotherm expression for VERSE).

2.2 Prediction of Cesium Loading

ZAM is an equilibrium multicomponent ion exchange model developed using several experimental and structure studies characterizing the ion exchange properties of hydrous crystalline silicotitanate in its powdered form (labeled as CST or IONSIV™ IE-910). It predicts the ion exchange equilibria of cesium and other cations in complex electrolytic solutions by solving the liquid-solid equilibrium and material balance equations for the cesium-CST system. The model includes the competitive ion exchange at CST exchange sites between multiple homovalent cations: Na^+, Cs^+, H^+, Rb^+, K^+, and $SrOH^+$. There are two different ways to estimate cesium loading: (1) Use of an isotherm, or (2) Variation of ZAM phase ratio.

- Use of an isotherm: An isotherm provides the equilibrium relation between the concentration of cesium loaded on the CST surface to the concentration of cesium in the solution. The isotherm covers a wide range of liquid-phase cesium concentrations. ZAM can generate equilibrium cesium loading data at a given temperature. Generally, an excellent fit for the ZAM data would be achieved by use of the Freundlich/Langmuir isotherm model.
- Variation of ZAM phase ratio: A phase ratio ϕ is defined as the ratio of total liquid volume (mL) processed to the mass of CST media (g_{CST}). To simulate cesium loading on a CST bed in the ion exchange column for a specified feed, ZAM calculations are performed at increasing phase ratios until the calculated equilibrium liquid cesium concentration approximates (usually accurate up to 4 digits) the feed cesium concentration. The resulting cesium concentration on CST represents the maximum cesium loading for that condition (Hang et al., 2017).

The two approaches should deliver practically identical results. Also, to account for inert binder and other less well-defined effects in the IX columns, a correction/dilution factor is applied to equilibrium cesium loading on CST for waste solutions. A description of the dilution factor was provided in a previous report (Hang et al., 2017).

2.3 Ion Exchange Column Model

The mathematical model utilized in the IX column simulations is a porous particle model that accounts for competitive adsorption (i.e., $Cs^+ >> K^+ > Na^+$), bulk advection, axial dispersion, film mass transfer, and pore diffusion. The numerical solutions of the governing equations and boundary conditions are performed by the VERSE-LC simulation package. The pore diffusion assumes uniform spherical adsorbent particles, plug flow with constant linear velocity, local equilibrium with the adsorbent, and constant diffusivities.

Early column performance (the first 5 to 10 bed volumes) may require the use of a multi-component model, but this is unnecessary for this application. Long-term performance should be adequately handled using the single-component formulation as discussed below (Hamm et al., 2001).

In this model the kinetics associated with local ion exchange at an active site are assumed to be very fast (faster than the various liquid mass transfer mechanisms that transport ions to that site). Assuming radial effects to be negligible within the active region of the packed bed (i.e., a large column-to-particle diameter ratio), a one-dimensional solute transport equation for the mobile phase becomes

$$\underbrace{\frac{\partial C}{\partial t}}_{\textbf{storage}} = \underbrace{E_b \frac{\partial^2 C}{\partial z^2}}_{\textbf{axial dispersion}} \underbrace{- u_o \frac{\partial C}{\partial z}}_{\textbf{advection}} \underbrace{- \frac{3(1-\varepsilon_b)k_f}{R_p \varepsilon_b}(C - C_{p,r=R_p})}_{\textbf{liquid film diffusion (mass transfer)}}$$

With boundary and initial conditions

z = 0: $E_b \frac{\partial C}{\partial z} = u_o (C(t,0) - C_o)$

z = L: $\frac{\partial C}{\partial z} = 0$

t = 0: $C = C(0,z)$

C:	Concentration in bed fluid, mol/L
E_b:	Axial dispersivity, cm^2/min
u_o:	Linear interstitial velocity, cm/min
R_p:	Average particle radius, µm
ε_b:	Bed porosity
k_f:	Liquid film mass transfer coefficient, cm/min
L:	Axial length of active bed of column, cm

Assuming uniformly sized spherical particles with a homogeneous distribution of pores, a one-dimensional species transport equation for the pore phase (within an average sized particle of media) becomes

$$\underbrace{\varepsilon_p \frac{\partial C_p}{\partial t}}_{\textbf{storage}} + \underbrace{(1-\varepsilon_p)\left(\frac{\partial Q}{\partial C_p}\right)\frac{\partial C_p}{\partial t}}_{\textbf{surface adsorption}} = \underbrace{\varepsilon_p \frac{D_p}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial C_p}{\partial r})}_{\textbf{Fickian pore diffusion}}$$

Subjected to boundary and initial conditions

r = 0: $\frac{\partial C_p}{\partial r} = 0$

r = R_p: $\varepsilon_p D_p \frac{\partial C_p}{\partial r} = k_f (C - C_{p,r=R_p})$

t = 0: $C_p = C_p(0,r)$

C_p:	Concentration in pore fluid, mol/L
Q:	Solid-phase solute concentration, mol/L_{Bed}
ε_p:	Particle porosity
D_p:	Pore diffusion coefficient, cm^2/min

2.4 Software and Quality Assurance

The overall TCCR work was requested under a Technical Task Request (Fellinger 2018). The work scope is described with the associated Task Technical and Quality Assurance Plan (King 2018).

The OLI Studio™ is an acquired software that meets the commercial grade definition criteria in accordance with Manual E7 Procedure 3.46 and is accepted from the vendor by verifying the parts identifiers are correct. Dedication of the commercial grade software in accordance with Manual E7, Procedure 5.07 is not required for the OLI software, which was classified as Level D (Choi 2001). All the activities related to the verification and validation of the OLI software database and the resulting models were documented in accordance with Manual E7 Procedure 5.40, Software Testing, Acceptance and Turnover.

SRNL was provided with two executable files (i.e., "CSTIEXV4.EXE" and "Cstiexv5.exe") of the ZAM program running on the PC platform. Version "Cstiexv5" includes some improvement to better account for strontium effect. It is however numerically less stable than version "CSTIEXV4". ZAM was developed to function under MS Windows XP and older versions of Windows. For newer Windows version (e.g., Windows 7, Windows 10), emulators are required to provide XP functionalities for ZAM to run. Without emulators, ZAM will not run in Windows versions newer than Windows XP. ZAM is currently classified as Level D software (Tamburello 2011). The functional requirements placed on ZAM Versions 4 and 5 were verified and validated (Hamm et al., 2001).

Prior to applying VERSE-LC to the ion exchange modeling a verification process was completed and the results of that effort were reported in Hamm et al. (1999). The verification process ensures that the installed Windows version of VERSE-LC (i.e., version 7.80) was capable of adequately solving the above-mentioned governing equations and provided guidelines on how to accurately use the VERSE-LC code (e.g., mesh refinement requirements and input/output options). For all column simulations, numerical errors associated with the results of VERSE-LC should be very small when compared to the uncertainties associated with various model input parameters (bed density, particle size, pore diffusion, etc.). VERSE-LC was classified as Level D (Hang 2017).

Note that all software (OLI, ZAM, and VERSE-LC) are classified as Level D. Therefore, they cannot be used for safety-related calculations. The customer specified that the applicable Quality Assurance classification for the modeling efforts is Production Support; Level D software is compliant with these requirements. No variability or uncertainty were included in the calculations.

3.0 Preliminary Calculations

In these preliminary calculations, the impacts of different parameters (e.g., feed solution, column configuration, temperature, flow rate, and particle size) on TCCR column performance were studied. The feed solutions of varying compositions considered in this study are: (1) SRS average simulant (Walker 1999), (2) Tank 10H Projected based on OLI modeling of Tank 10H Salt Cake Core samples (Martino et al., 2004), and (3) Tank 10H Adjusted VDS based on characterization data and adjustment to 6 M Na^+ (Reboul 2017). Waste compositions of the evaluated feeds are shown in Table 1. Strontium was included in Tank 10H Adjusted VDS but at a concentration that is not expected to influence performance significantly. Note that these projected feed compositions are much higher in total sodium ion molarity than the recently measured concentrations for Batch 1A (Taylor-Pashow et al., 2019c) discussed in Section 4.0.

Table 1. Waste Compositions of the Evaluated Feeds

	SRS Average Simulant (Walker 1999)	**Tank 10H Projected** (Martino et al., 2004)	**Tank 10H Adjusted VDS** (Reboul 2017)
Component	Concentration (M)		
Na^{+1}	5.6	6.97	6
K^{+1}	0.015	0.0214	0.0062
Cs^{+1}	$1.4x10^{-5}$	$2.16x10^{-5}$	$2.9x10^{-5}$
Ca^{+2}	---	---	$5.6x10^{-5}$
Sr^{+2}	---	---	$8.9x10^{-7}$
OH^{-1}	1.94	0.373	0.34
NO_3^{-1}	2.14	4.28	1.96
NO_2^{-1}	0.52	0.139	0.24
$Al(OH)_4^{-1}$	0.31	0.0174	0.118
CO_3^{-2}	0.16	0.125	0.95
SO_4^{-2}	0.15	0.966	0.71
Cl^{-1}	0.025	---	0.0076
F^{-1}	0.032	---	0.0099
PO_4^{-3}	0.01	---	0.0021
OLI Density (g/cm3)	1.250 (25ºC)	1.327 (35ºC)	1.279 (35ºC)
	1.249 (35ºC)		
OLI Viscosity (cP)	2.78 (25ºC)	2.494 (35ºC)	2.675 (35ºC)
	2.20 (35ºC)		

Table 2 summarizes the CST bed properties and TCCR column design parameters used in the VERSE-LC preliminary calculations. The values within brackets are recommended later, based on more recent CST modeling studies. Again, the primary goal of the preliminary calculations was to evaluate the variation of different parameters on the column performance.

Table 2. CST Bed Properties and TCCR Column Design

Properties	Values
CST Form	Na^+
Bed Density (g/ml_{bed})	1.05 (*)
F-Factor	0.82 [0.89]
Dry Bed Density (g_{CST}/ml_{bed})	0.861 [0.935]
Bed Porosity	0.5 [0.548]
Particle Porosity	0.24
Particle Diameter (µm)	344 (SCIX) (**) 572 (TCCR)
Particle Tortuosity	5 [4]
Bed Diameter (cm)	48.68
Bed Length (cm)	263.59
Bed Volume (gal)	129.6
Column Head Space (gal)	15.85

[]: Parameters recommended by L. L. Hamm based on recent CST modeling studies
(*): UOP analysis (UOP 2017)
(**): Historical particle diameter used for the Small Column Ion Exchange vs. the 572 µm measured for TCCR batch of media

The cases evaluated are listed in

Table 3. These cases are characterized by the following parameters:

1. Configuration: single column, or 3 columns in series (i.e., lead-lag-guard)
2. Feed solution: SRS average, Tank 10H Projected, and Tank 10H Adjusted VDS
3. Temperature (°C): 25, or 35
4. Flow rate (gpm): 2, 3, 5, or 8
5. Particle size diameter (µm): 344, or 572

Table 3. Preliminary Evaluation Cases

Cases	Columns	Feed [*]	T (°C)	Flow Rate (gpm)	Particle Size (μm)
1a	Single	SRS Avg	35	5	344
1b	Single	SRS Avg	35	8	344
1c	Single	SRS Avg	35	10	344
1d	Single	SRS Avg	25	5	344
1e	Single	SRS Avg	35	5	572
1f	Single	Tank 10 Projected	35	5	572
2a	Single	SRS Avg	35	3	572
2b	3 Columns	SRS Avg	35	3	572
2c	3 Columns	SRS Avg	35	5	572
2d	3 Columns	SRS Avg	35	8	572
2e	3 Columns	SRS Avg	35	2	572
2f	3 Columns	Tank 10H Projected	35	2	572
2g	3 Columns	Tank 10H Adj. VDS	35	2	572
3a	3 Columns	SRS Avg	35	5 (up to 500 BVs) 2 (after 500 BVs)	572

[*]: SRS Average Simulant (Walker 1999); Tank 10H Projected (Martino et al., 2004); Tank 10H Adj. VDS (Reboul 2017)

Adsorption isotherms for the feed solutions were determined by use of the Freundlich/Langmuir Hybrid model to fit the ZAM equilibrium data. The isotherm parameters are given in Table 4. With the parameters listed, the expression reduces to a Langmuir isotherm. A binder correction/dilution factor of 0.68 was applied to cesium loading on the engineered CST form in the TCCR columns; subsequent calculations varied this value to obtain better agreement of predictions with measurements.

$$Q = \frac{\eta_{CF} C_T \rho_{Bed} C_p^{M_a}}{\beta + b C_p^{M_b}}$$

Q: Cesium loading on CST (mol_{Cs}/L_{Bed})
C_p: Liquid-phase cesium concentration (mol_{Cs}/L)
C_T: Total cesium capacity of resin ($mmol_{Cs}/g_{CST}$)
η_{CF}: Correction/dilution factor
ρ_{Bed}: Dry bed density (g_{CST}/mL_{Bed})
β: Selectivity parameter (mol_{Cs}/L)

The β parameter for cesium, containing the selectivity coefficients, depends upon temperature and liquid composition of all ionic species in solution. Hence, different waste solutions should have different β values. The loading equation indicates that the cesium loading increases with decreasing β. Note that the cesium loading Q expression (mol_{Cs}/L_{Bed}) is formulated to be used in VERSE-LC. The equilibrium cesium loading ($mmol_{Cs}/g_{CST}$) shown in many equilibrium isotherm figures in this report was determined from ZAM.

Table 4. Isotherm Parameters

Feed (*)	T (°C)	η_{CF}	C_T ($mmol_{Cs}/g_{CST}$)	ρ_{Bed}	M_a	M_b	β	b
SRS Avg	25	0.68	0.58	0.861	1	1	2.42E-04	1
SRS Avg	35	0.68	0.58	0.861	1	1	3.12E-04	1
Tank 10 Projected	35	0.68	0.58	0.861	1	1	8.10E-04	1
Tank 10 Adj. VDS	35	0.68	0.58	0.861	1	1	2.56E-04	1

(*): SRS Average Simulant (Walker 1999); Tank 10H Projected (Martino et al., 2004); Tank 10H Adj. VDS (Reboul 2017)

For comparison, the isotherms for the feed solutions are displayed in Figure 2. In general, cesium loading increases with decreasing temperatures. Compared to SRS Average simulant, less loading would be expected with the Tank 10H Projected composition primarily due to the decreased OH^- concentration and increased K^+ content. The Tank 10H Adjusted VDS isotherm should be higher than the SRS Average simulant isotherm because of a large increase (i.e., a 2x increase) in cesium concentration in the former despite the higher Na^+ concentration. These trends are confirmed by the isotherm plots in Figure 2.

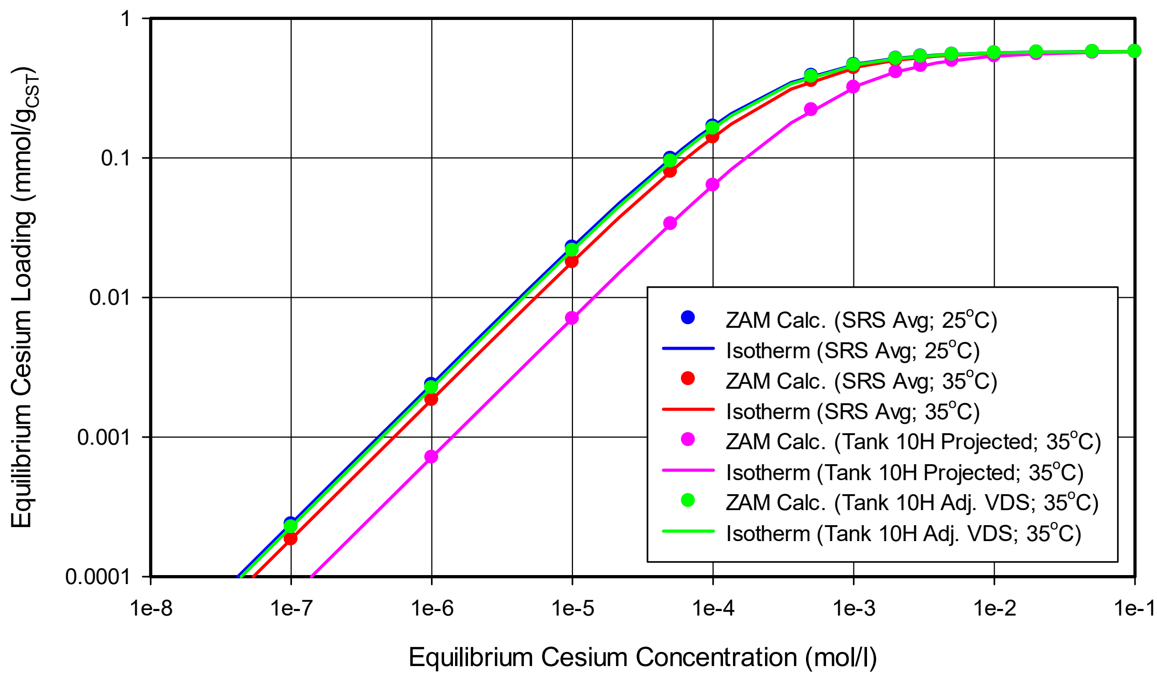

Figure 2. Equilibrium Isotherms

In each simulation case, the goal was to determine the waste solution in term of bed volumes (BVs) processed through TCCR, and the CST bed utilization in the lead column at the breakthrough of decontamination factor (DF) of 1000. The breakthrough can be based on either the effluent concentration or the bucket-average concentration. Bucket-average concentration delays the breakthrough because it is based on a volume-average concentration. As examples, the breakthrough and the CST bed utilization were shown for Case 1a (single column) in Figure 3 and Figure 4, and Case 2b (three columns) in Figure 5 and Figure 6. In Figure 6, the lead-column (column 1) cesium concentrations profiles are provided at the breakthrough for three different column configurations (i.e., 1, 2, or 3 columns). Note that as expected in Case 2b the lead column bed utilization result for the single-column configuration is identical to the result of Case 2a. Figure 6 clearly shows that the lead column CST bed is best utilized (91.4 %) in a lead-lag-guard configuration. The result figures for all evaluation cases are provided in Appendix A.

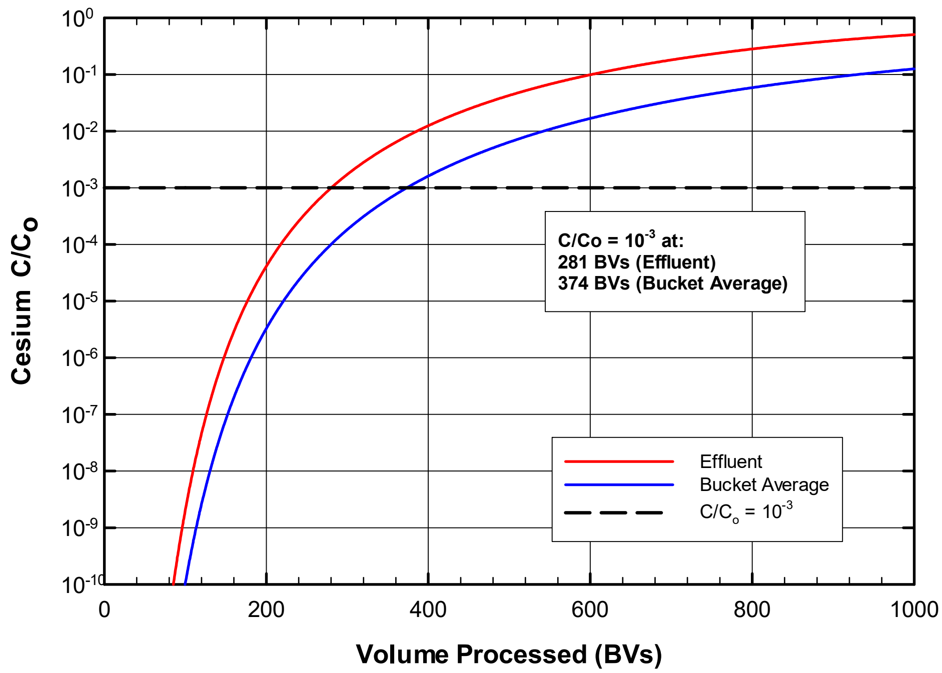

Figure 3. Case 1a Breakthrough Curves

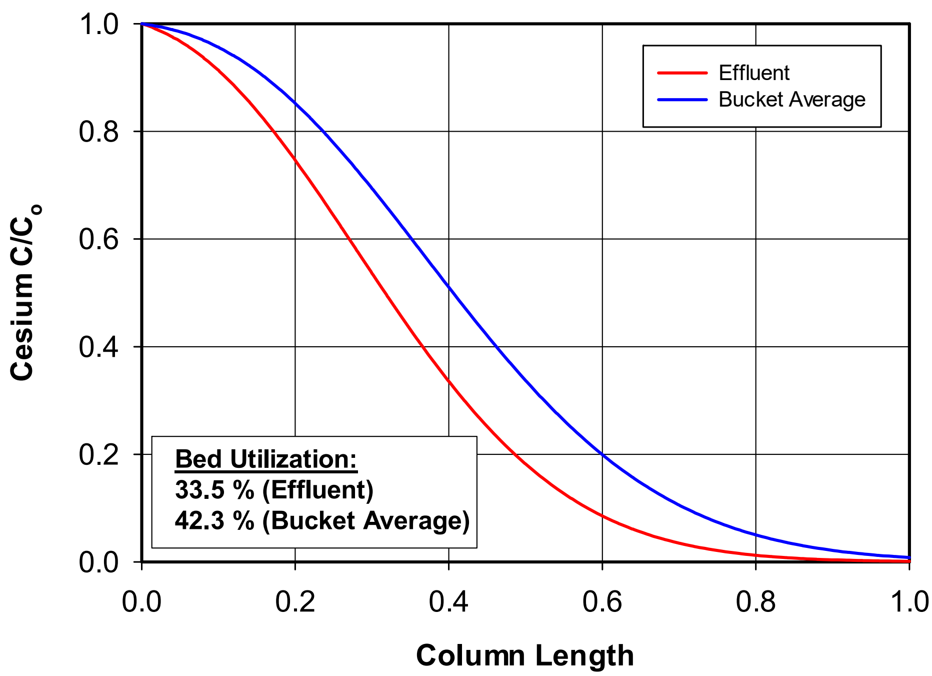

Figure 4. Case 1a Column Concentration Profiles

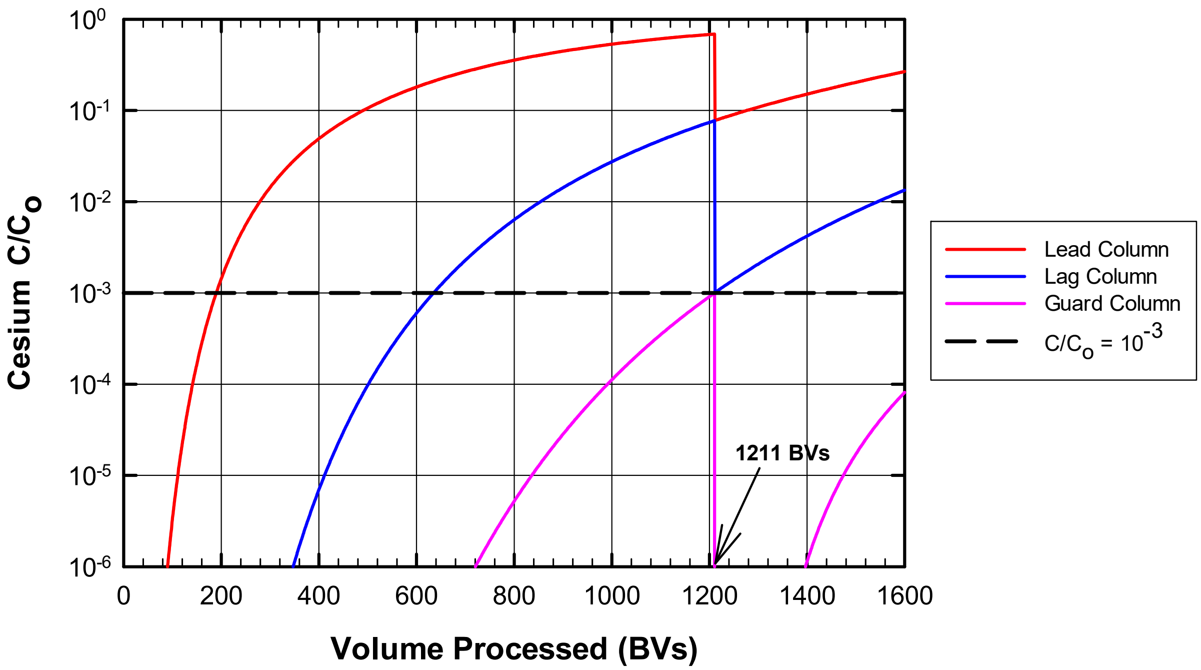

Figure 5. Case 2b Breakthrough Curves

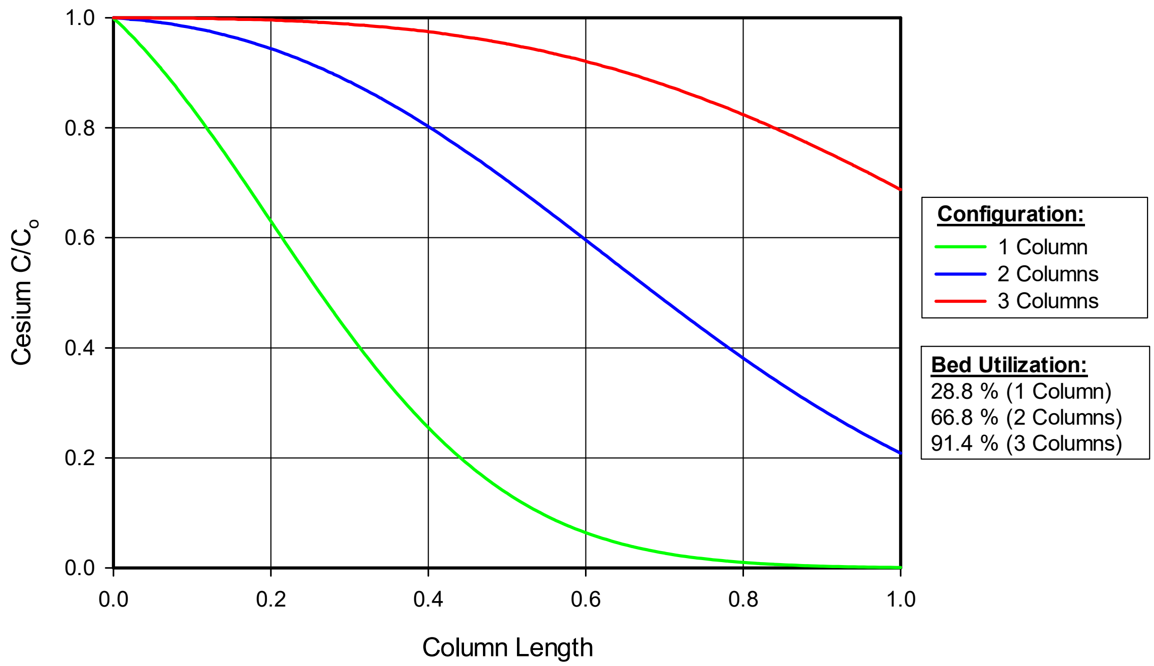

Figure 6. Case 2b Lead Column Concentration Profiles at Breakthrough

The preliminary cases were performed using VERSE-LC and the results are summarized in Table 5. Regarding the specified column head space, for single- and two-column configurations, the VERSE results with and without column head space are practically identical. For the three-column configuration, VERSE showed some numerical anomaly in the guard-column effluent concentration after the breakthrough of DF 1000 was reached and the rotation of columns took place. Therefore, in this study, for simplification, all VERSE calculations were carried out without column head space. VERSE input and output files for all preliminary cases are provided in Appendix B.

Overall, the VERSE results in Table 5 show the following findings:

- TCCR performance (i.e., amount of waste solutions processed) is improved:
  - At slower flow rates and lower operating temperatures
  - With smaller CST particle sizes
- Single column configuration does not utilize the CST bed effectively, showing at best a low utilization of 33.5 % (based on effluent concentration at column outlet) or 42.3 % (based on bucket-average concentration). Hence, multi-column serial configurations are recommended.
- Newer parameters based on more recent CST modeling studies deliver more favorable results.

Table 5. Results of the Preliminary Calculations

Cases	Columns	Feed [a]	T (°C)	Flow Rate (gpm)	Particle Size (μm)	BVs at DF = 1000 [b]	Bed Utilization at DF = 1000 [b] (%)
1a	Single	SRS Avg	35	5	344	281 [374]	33.5 [42.3]
1b	Single	SRS Avg	35	8	344	199 [272]	29.2 [36.4]
1c	Single	SRS Avg	35	10	344	166 [229]	28.0 [34.5]
1d	Single	SRS Avg	25	5	344	349 [466]	33.0 [41.8]
1e	Single	SRS Avg	35	5	572	123 [173]	26.4 [32.4]
1f	Single	Tank 10H Projected	35	5	572	37 [52]	25.5 [31.1]
2a	Single	SRS Avg	35	3	572	190.3 [261.6]	28.8 [35.8]
2b	3 Cols	SRS Avg	35	3	572	1211	91.4 [c]
2c	3 Cols	SRS Avg	35	5	572	896	80.3 [c]
2d	3 Cols	SRS Avg	35	8	572	641	71.7 [c]
2e	3 Cols	SRS Avg	35	2	572	1467 1666 [d]	97.3 [c] 98 [c], [d]
2f	3 Cols	Tank 10H Projected	35	2	572	498 570 [d]	93 [c] 94.8 [c], [d]
2g	3 Cols	Tank 10H Adj. VDS	35	2	572	1468	93 [c]
3a	3 Cols	SRS Avg	35	5 (up to 500 BVs) 2 (after 500 BVs)	572	1183	89.3 [c]

[a]: SRS Average Simulant (Walker 1999); Tank 10H Projected (Martino et al., 2004); Tank 10H Adj. VDS (Reboul 2017)
[b]: Based on column effluent concentration; []: Based on bucket-average concentration
[c]: Lead column bed utilization at guard column DF = 1000
[d]: Parameters recommended by L. L. Hamm based on more recent CST modeling studies

4.0 Tank 10H Batch 1 and Batch 1A Operations

As discussed under Section 1.1, Tank 10H serves dual functions as both the salt dissolution tank as well as the feed tank for the TCCR system. Prior to the operation of TCCR, Tank 10H undergoes dissolution campaigns, dissolving the salt cake to form an aqueous salt solution (i.e., supernate). For Batch 1, well water (~150,000 gallons) was added to Tank 10H, and the contents were recirculated. After more than 7 days of recirculation, surface samples were obtained and sent to SRNL for analysis (Taylor-Pashow et al., 2019a). Analysis results indicated minimal dissolution of the salt had occurred, and that chemical adjustment of the supernate would be required to process this batch through the TCCR columns. Therefore, ~16,870 gallons of 50 wt% NaOH was added to Tank 10H and the contents were mixed by recirculation to form Batch 1A. The target of this adjustment was to increase the Na^+ concentration to at least 3.5 M. After ~4 days of recirculation, samples were taken from the tank, and sent to SRNL for analysis (Taylor-Pashow et al., 2019b). Additionally, in each batch, the in-tank CST batch contact equilibrium (or "teabag") samples were collected and analyzed. The teabag samples refer to a test where a small amount of CST was placed in a special container lowered every two days into the tank that remained submerged in the unagitated liquid over a 10-day period. The cesium-loaded CST was retrieved from the tank and analyzed by SRNL. At about the same time, traditional CST batch contact tests were conducted in SRNL under controlled conditions using Batch 1 and Batch 1A supernate samples (King et al., 2019a). Note that engineered form of CST from the same batch of IONSIV™ R9120-B as used in the TCCR columns was employed in both teabag and SRNL batch contact tests after preconditioning. ZAM equilibrium cesium loading calculations were compared with teabag and SRNL batch contact test data to obtain appropriate correction factors. VERSE-LC was utilized for predicting the TCCR performance to process Batch 1A supernate. Batch 1 and Batch 1A samples were analyzed and their OLI modeled supernate compositions are given in

Table 6. The bulk diffusivity is a required input to VERSE-LC. In the past, the cesium diffusivity in the bulk feed solution (free diffusivity) was calculated using the Nernst-Haskell equation (Smith, 2011). In this study, for consistency, the cesium bulk diffusivity, as other properties (i.e., density, viscosity, equilibrium compositions), was obtained from OLI.

Table 6. Batch 1 and Batch 1A Supernate Compositions

Component	Batch 1 (Taylor-Pashow et al., 2019a)	Batch 1A (Taylor-Pashow et al., 2019b)
Na^{+1}	2.02	3.79
K^{+1}	$1.84x10^{-3}$	$2.21x10^{-3}$
Cs^{+1}	$1.1719x10^{-5}$	$1.13x10^{-5}$
$SrOH^{+1}$	$3.0484x10^{-8}$	$1.6263x10^{-7}$
Sr^{+2}	$1.3652x10^{-7}$	$4.6971x10^{-8}$
Ca^{+2}	---	$7.14x10^{-5}$
Fe^{+3}	---	$4.99x10^{-5}$
OH^{-1}	0.235	1.82
NO_3^{-1}	0.714	0.727
NO_2^{-1}	0.0743	0.0755
$Al(OH)_4^{-1}$	0.0413	0.0422
CO_3^{-2}	0.292	0.322
SO_4^{-2}	0.131	0.174
Cl^{-1}	0.11125 (1)	0.12727 (2)
F^{-1}	0	0
PO_4^{-3}	0	0
$C_2O_4^{-2}$	---	0.00427
OLI Diffusivity (cm^2/min)	---	$7.9343x10^{-4}$ (34 °C)

(1): measured concentration was < 8.4E-03 M, Cl^{-1} adjusted for charge balance
(2): measured concentration was 6.6E-03 M, Cl^{-1} adjusted for charge balance

4.1 Tank 10H Teabag Tests and SRNL Batch Contact Tests

Tank 10H temperature was initially estimated by SRR process engineers to be ~38 ^oC. Therefore, the ZAM loading calculations were performed at 38 ^oC for Batch 1 (Taylor-Pashow et al., 2019a). Likewise, SRNL batch contact tests were conducted at 38 ^oC for both Batch 1and Batch 1A samples. Upon completion of Batch 1 teabag tests, available data however indicated an actual tank temperature of ~34 ^oC. As a result, Batch 1A ZAM equilibrium cesium loading was calculated at 34 ^oC (Taylor-Pashow et al., 2019b). In this report, Batch 1 and Batch 1A ZAM cesium loading and VERSE-LC calculations are performed at 34 ^oC. Modeling of SRNL batch contact tests is performed at 38 ^oC to reflect the actual test condition.

Again, for the waste supernates of Batch 1 and Batch 1A, isotherms were determined by use of the Freundlich/Langmuir Hybrid model to fit the ZAM data. The Freundlich/Langmuir isotherm model was shown in Section 3.0 above and the isotherm parameters are listed in Table 7. For the listed parameters, the isotherm expression reduces to a Langmuir model.

Table 7. Batch 1 and Batch 1A Isotherm Parameters

Feed	T (°C)	η_{df}	C_T ($mmol_{Cs}/g_{CST}$)	M_a	M_b	β	b
Batch 1	34	0.68	0.58	1	1	6.9299E-05	1
Batch 1	38	0.68	0.58	1	1	7.7021E-05	1
Batch 1A	34	0.68	0.58	1	1	1.2358E-04	1
Batch 1A	38	0.68	0.58	1	1	1.3765E-04	1

4.1.1 Tank 10H Teabag Tests

For each feed supernate, the maximum cesium loading was calculated by the method of phase ratio variation (i.e., the liquid-to-solid phase ratio was increased until the initial and final Cs concentrations were almost identical). Cesium loadings at 34 °C at the feed concentration and batch composition are given in Table 8. The ZAM loading values that are in the powdered form are given in Column 2 of the table. For comparison with the teabag results, the ZAM values are converted to the engineered-form values using a common correction factor of 0.68 (Column 3). The predicted values (engineered form) are 3.1x and 2.7x larger than the teabag results for Batch 1 and Batch 1A, respectively.

Table 8. Maximum Cesium Loading at 34 °C

Supernate Samples	q (Powdered Form)(1) $mmol_{Cs}/g_{CST}$	q (Engineered Form)(2) $mmol_{Cs}/g_{CST}$	Teabag $mmol_{Cs}/g_{CST}$
Batch 1	0.0839	0.0571	0.0183
Batch 1A	0.0485	0.033	0.0122

(1): Calculated from ZAM; (2): Applied common correction/dilution factor η_{CF} of 0.68 to ZAM values

Cesium loading and isotherm with and without the binder correction/dilution factor are shown in Figure 7 for Batch 1 and in Figure 8 for Batch 1A. The figures show that much smaller correction factors (i.e., 0.218 for Batch 1 and 0.251 for Batch 1A) are required for the ZAM isotherms to adequately represent the test data. The reason for the difference between the ZAM calculated loadings and the teabag results was discussed in detail elsewhere (Taylor-Pashow et al., 2019a and 2019b). The most likely cause for the discrepancy between the modeling and experimental data remains competition or potential precipitation from other ions (e.g., Ca, Fe, Cr, Mg, Mn etc.) found on the CST. Further study would be necessary to better understand the cesium sorption mechanism in these chemistry regimes.

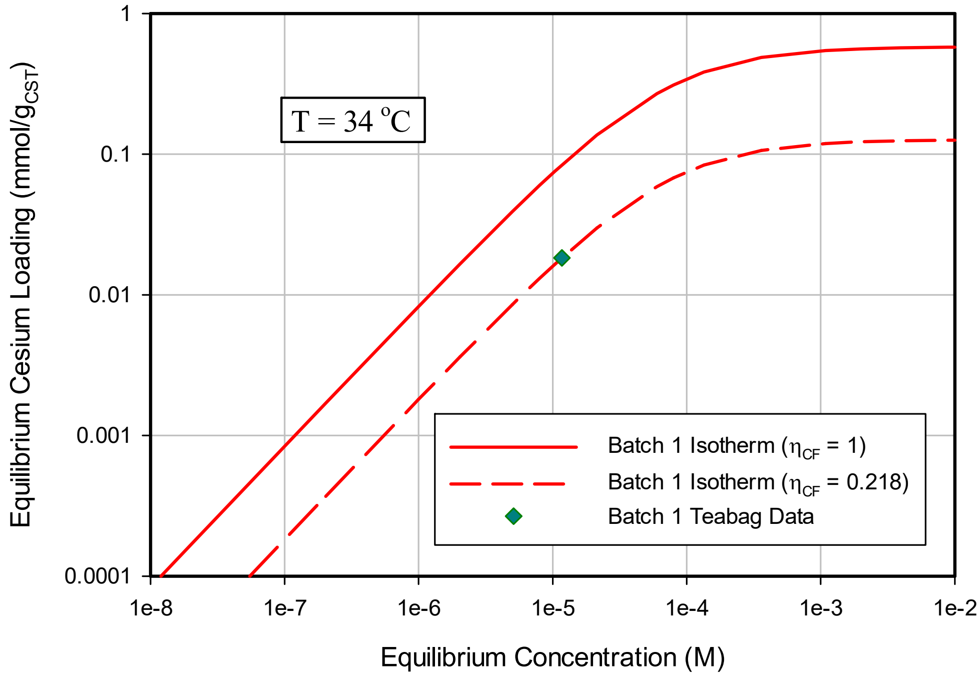

Figure 7. Batch 1 ZAM Cesium Loading Isotherms versus Teabag Results at 34 °C

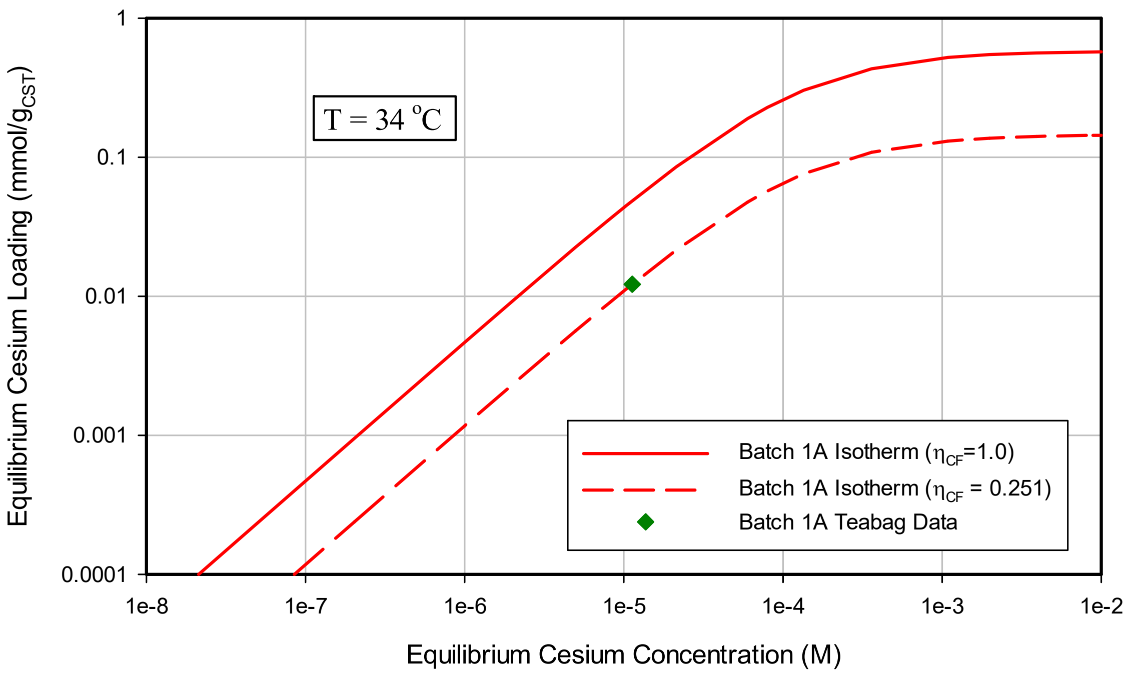

Figure 8. Batch 1A ZAM Cesium Loading Isotherms versus Teabag Results at 34 °C

4.1.2 SRNL Batch Contact Tests

As discussed in the previous section, cesium loading on the CST media in the teabag tests unexpectedly was much lower than ZAM isotherm model predictions. As a result, traditional CST batch contact tests were conducted at SRNL under controlled conditions using Tank 10H waste supernate samples collected from the tank for both Batch 1 and Batch 1A. The cesium equilibrium loading data from these SRNL tests was compared to the teabag results and ZAM model predictions. Detailed description of the batch contact tests was provided in a separate document (King et al., 2019a).

As in the teabag tests, the ZAM isotherm model was used to predict equilibrium cesium loading on CST during batch contact testing with Tank 10H Batches 1 and 1A supernate samples. A binder correction factor of 0.68 has typically been used to account for the contribution of binder materials to the mass of engineered CST media. A correction factor of 1 means no correction for binder dilution. In Figure 9, the final cesium concentration observed for Tank 10H Batch 1 did not fall on the equilibrium isotherm predicted for powdered form CST, as expected, because ZAM data is based on the powdered form. However, a correction factor of 0.531 was required to match the experimental results. This is 22 % below the binder correction/dilution factor used in previous testing with the same batch of media and indicates that CST cesium removal performance is lower than expected, though not as low as was observed for the teabag which was 68 % below the prediction for engineered form CST. Figure 10 shows that a correction factor of 0.464 was required to match the experimental results for Tank 10H Batch 1A supernate. This is 32 % below the typical 0.68 correction/dilution factor, indicating a lower CST cesium removal performance than expected, though not as low as was observed for the teabag which was 63 % below the prediction for engineered form CST. As mentioned above, the reason may be due to competitors and/or precipitation of solids.

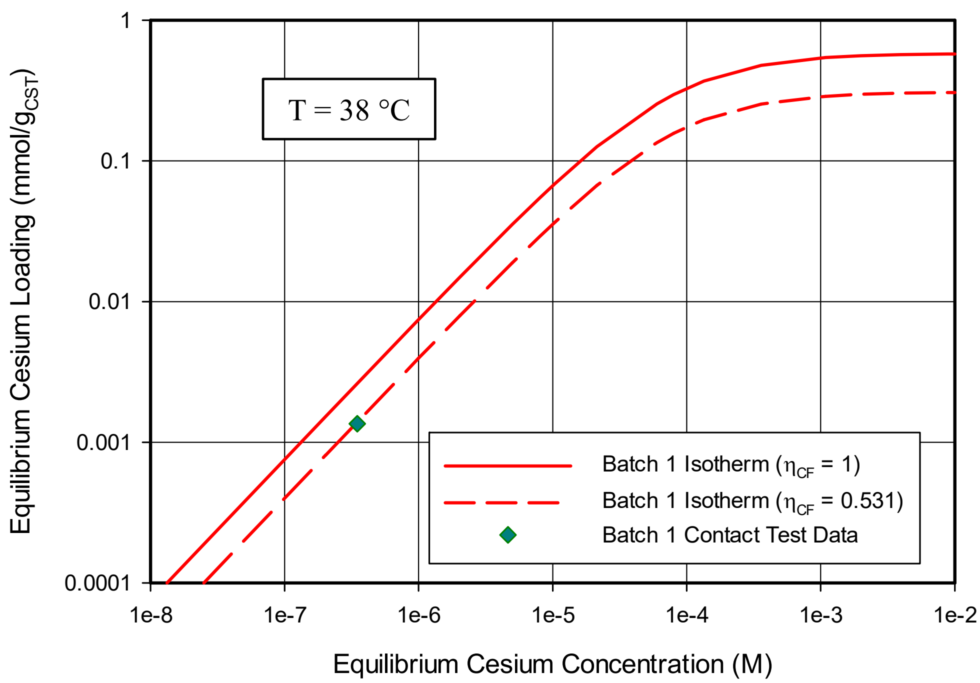

Figure 9. Batch 1 ZAM Cesium Loading Isotherms versus Batch Contact Results at 38 °C

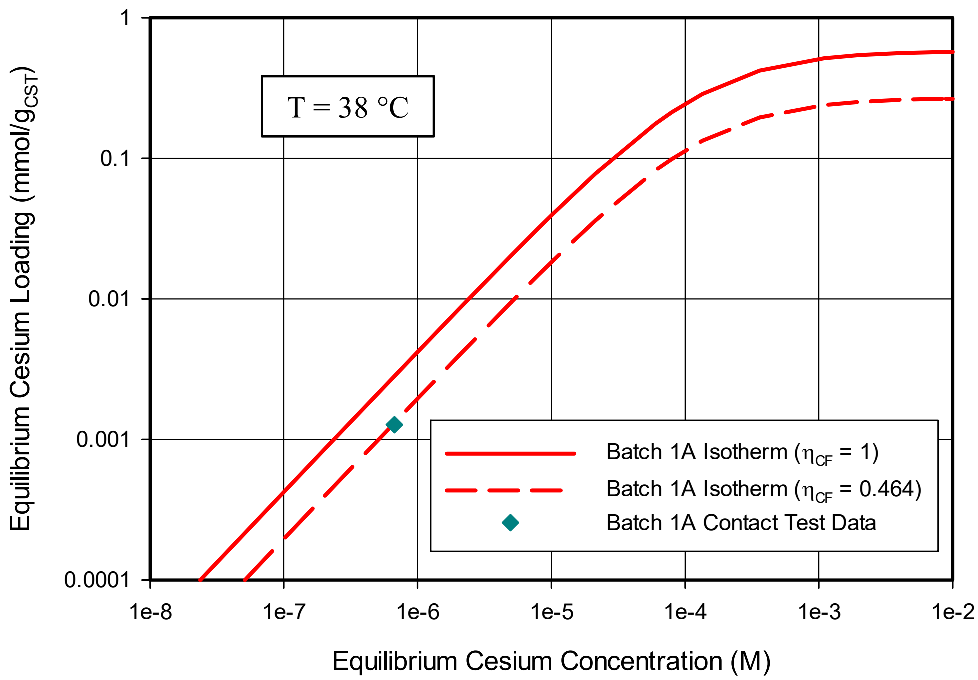

Figure 10. Batch 1A ZAM Cesium Loading Isotherms versus Batch Contact Results at 38 °C

4.1.3 VERSE-LC Calculations for TCCR Batch 1A Operations

With Batch 1A content in Tank 10H ready to be processed through the TCCR system, VERSE-LC was utilized to predict the TCCR column performance in several operational scenarios. The cases of interest shown in Table 9 evaluate the impact of column configurations, correction/dilution factor, and flow rates on the TCCR column performance. In addition to the traditionally used value of 0.68, correction factors of 0.251 and 0.464 determined from Tank 10H Batch 1A teabag and SRNL batch contact tests, respectively, are used. Although 0.464 was obtained from the batch contact tests at 38 °C, it is assumed that correction factor insignificantly changes with temperature. Correction factors of 0.251 and 0.68 provide lower and upper bound performance results.

Table 9. Evaluation Cases of Batch 1A TCCR Operation at 34 °C

Cases	Columns	Correction Factor η_{CF}	Flow Rate (gpm)
5a	2 Columns	0.464	5
5b	3 Columns	0.464	3
5c	2 Columns	0.251	5
5d	3 Columns	0.251	3
5e	2 Columns	0.68	5
5f	3 Columns	0.68	3

A summary of the parameters used in the VERSE-LC calculations is provided in Table 10. These updated values were taken from the batch contact test memo (King et al., 2019a) and the recent kinetics study report for this specific batch of media (King et al., 2019b).

Table 10. Updated CST Bed Properties

Properties	Values
Bed Density (g/ml_{bed})	1.2097
F-Factor	0.8177
Dry Bed Density (g_{CST}/ml_{bed})	0.9892
Bed Porosity	0.548
Particle Porosity	0.24
Particle Diameter (μm)	572
Particle Tortuosity	4

The Batch 1A operational scenarios were simulated using VERSE-LC and the results are given in Table 11. VERSE input and output files for Batch 1A predictions are listed in Appendix B. As shown in Table 11, breakthroughs are provided based on both effluent concentration and bucket-average concentration. These volumes are much larger than the breakthrough predictions for SRS Average simulant composition because of the much lower Na^+ and K^+ concentrations. As previously discussed under Section 3.0, due to the accumulation effect, the bucket-average concentration criterion delays the column breakthrough because it is based on a volume-average concentration. As an example, Figure 11 displays the breakthroughs in Case 5c based on both criteria of instantaneous effluent concentration and bucket-average concentration. A complete graphical set of the VERSE-LC results for Batch 1A is given in Appendix A.

The operating data of the TCCR Batch 1A for the 2-column (lead-lag) configuration shows a total processed waste volume of ~1,080 BVs, i.e., much larger than the VERSE-LC results using correction factor of 0.251 (Case 5c in Table 11).

More data should be available soon from TCCR operation and/or potentially from column testing under controlled laboratory conditions for validation of the VERSE-LC column performance predictions. It is essential that VERSE-LC be favorably compared to operational/test data for SRNL to better assist SRR in future TCCR operations.

Table 11. VERSE-LC Results for Batch 1A TCCR Operation at 34 °C

Cases	BVs at First DF Breakthrough [(a)]
5a	1352 [1763]
5b	3169 [3863]
5c	733 [955]
5d	1715 [2091]
5e	1981 [2584]
5f	4644 [5660]

[(a)]: Based on column effluent concentration
[]: Based on bucket-average concentration

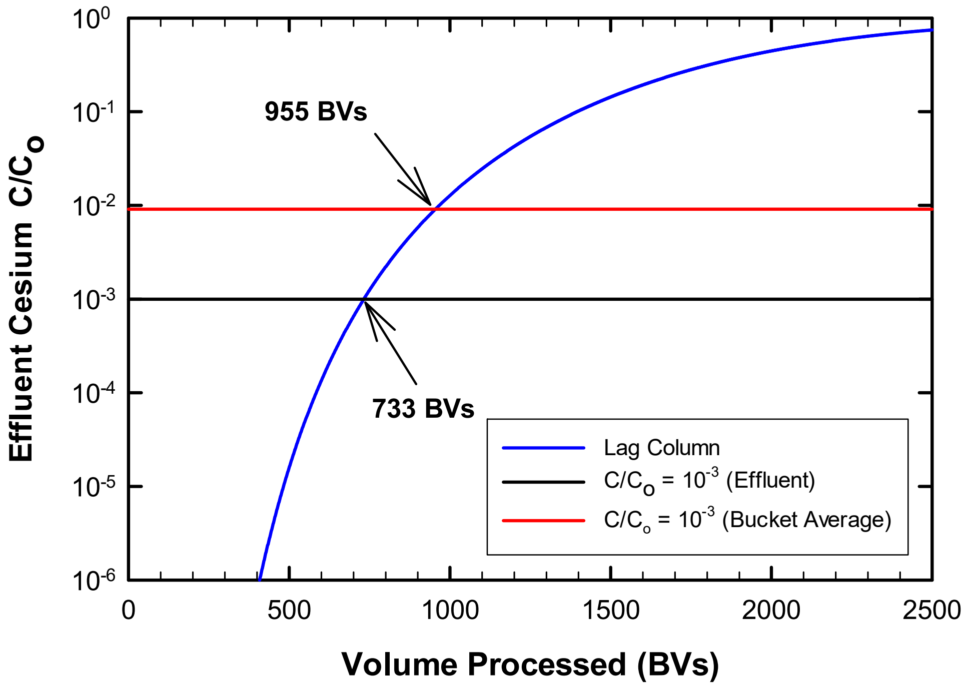

Figure 11. Case 5c Breakthrough Curves

5.0 Conclusions

VERSE-LC was applied to predict TCCR column performances. The preliminary calculations indicate:

- TCCR performance is improved at slower process flow rate, at lower operating temperature, and with smaller CST particle size.
- Multi-column configurations are highly recommended, because single column configuration does not utilize the CST bed effectively.

In addition to the traditionally used value of 0.68, binder correction/dilution factors were determined to be 0.251 based on the Tank 10H teabag tests and 0.464 based on SRNL batch contact tests. Therefore, binder correction factors of 0.251 and 0.68 would provide lower and upper bound performance results, respectively. These lower binder correction factors are potentially due to competing ions and/or precipitation of solids.

To better assist SRR in future TCCR operations, it is essential to validate VERSE-LC predictions using operational/test data. It is also necessary to further investigate the cause of the much lower binder dilution/correction factor for the teabag and batch contact testing. The results suggest there may be unknown competitor(s) or precipitant(s) that potentially interfere with the adsorption of cesium, which can substantially impact the effectiveness and cost of future use of CST.

6.0 References

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Appendix A. Results for All Evaluation Cases

Table A-1. List of Evaluation Cases

Cases	Columns	Correction Factor η_{CF}	Feed (*)	T (°C)	Flow Rate (gpm)	Particle Size (µm)
1a	1	0.68	SRS Avg	35	5	344
1b	1	0.68	SRS Avg	35	8	344
1c	1	0.68	SRS Avg	35	10	344
1d	1	0.68	SRS Avg	25	5	344
1e	1	0.68	SRS Avg	35	5	572
1f	1	0.68	Tank 10 Projected	35	5	572
2a	1	0.68	SRS Avg	35	3	572
2b	3	0.68	SRS Avg	35	3	572
2c	3	0.68	SRS Avg	35	5	572
2d	3	0.68	SRS Avg	35	8	572
2e	3	0.68	SRS Avg	35	2	572
2f	3	0.68	Tank 10H Projected	35	2	572
2g	3	0.68	Tank 10H Adj. VDS	35	2	572
3a	3	0.68	SRS Avg	35	5 (up to 500 BVs) 2 (after 500 BVs)	572
5a	2	0.464	Batch 1A	34	5	572
5b	3	0.464	Batch 1A	34	3	572
5c	2	0.251	Batch 1A	34	5	572
5d	3	0.251	Batch 1A	34	3	572
5e	2	0.68	Batch 1A	34	5	572
5f	3	0.68	Batch 1A	34	3	572

(*): SRS Average Simulant (Walker 1999); Tank 10H Projected (Martino et al., 2004); Tank 10H Adj. VDS (Reboul 2017); Batch 1A (Taylor-Pashow et al., 2019b)

Case 1a

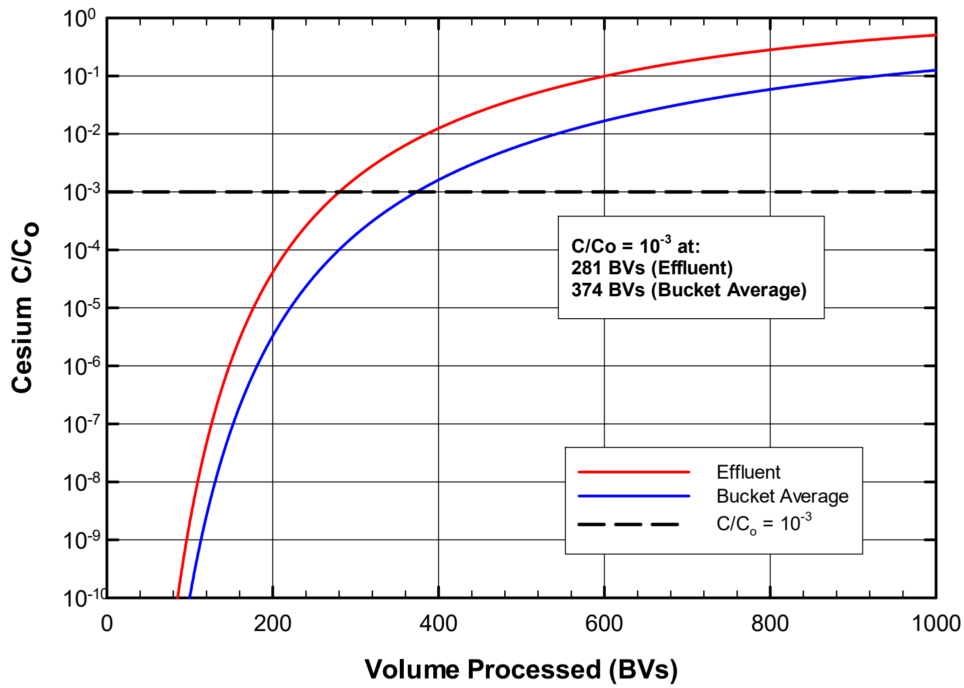

Figure A-1. Case 1a Breakthrough Curves

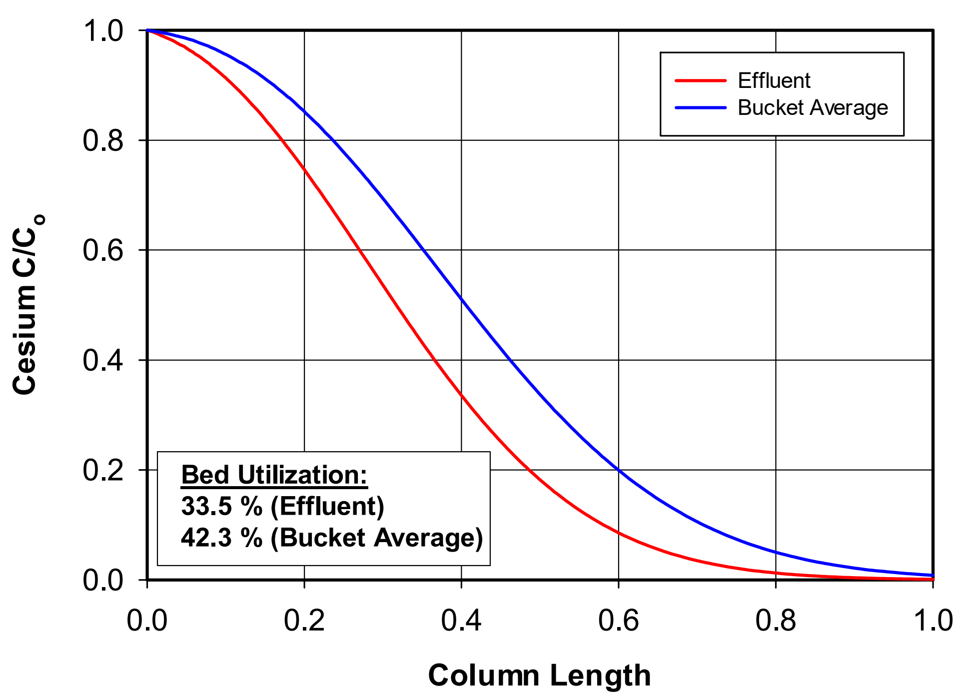

Figure A-2. Case 1a Column Concentration Profiles

Case 1b

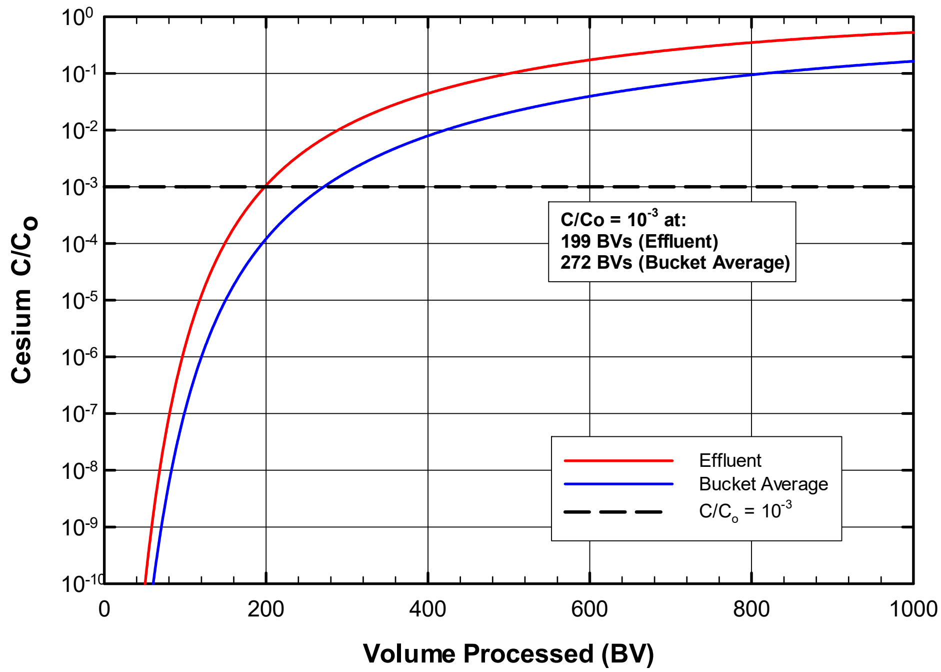

Figure A-3. Case 1b Breakthrough Curves

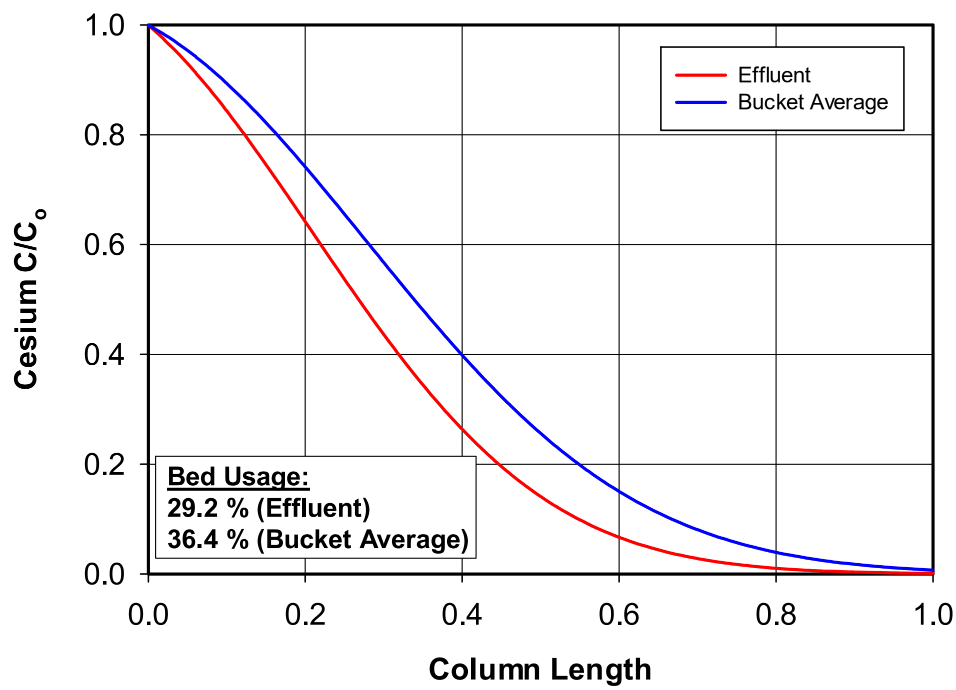

Figure A-4. Case 1b Column Concentration Profiles

Case 1c

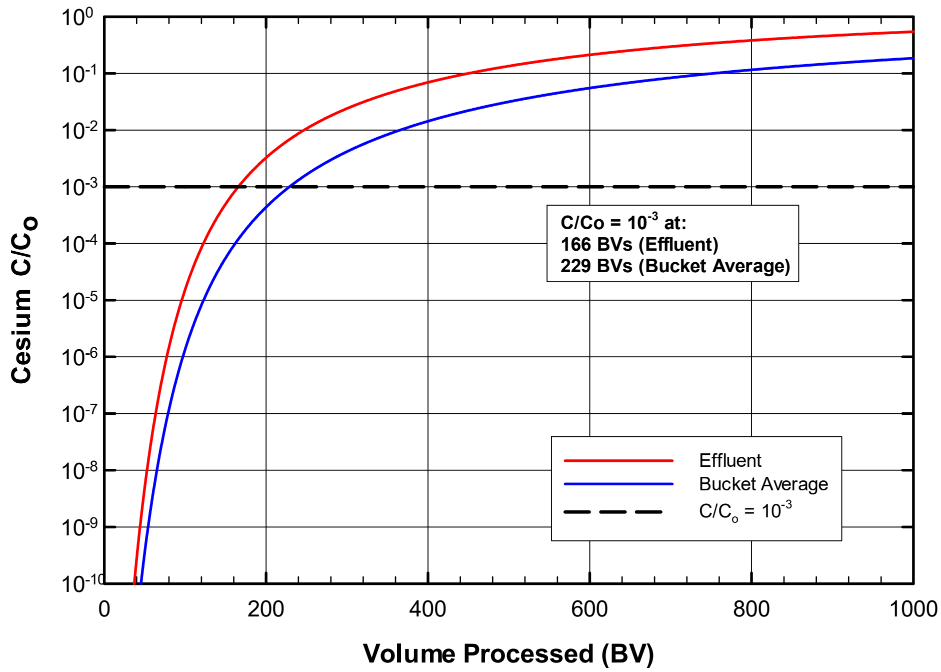

Figure A-5. Case 1c Breakthrough Curves

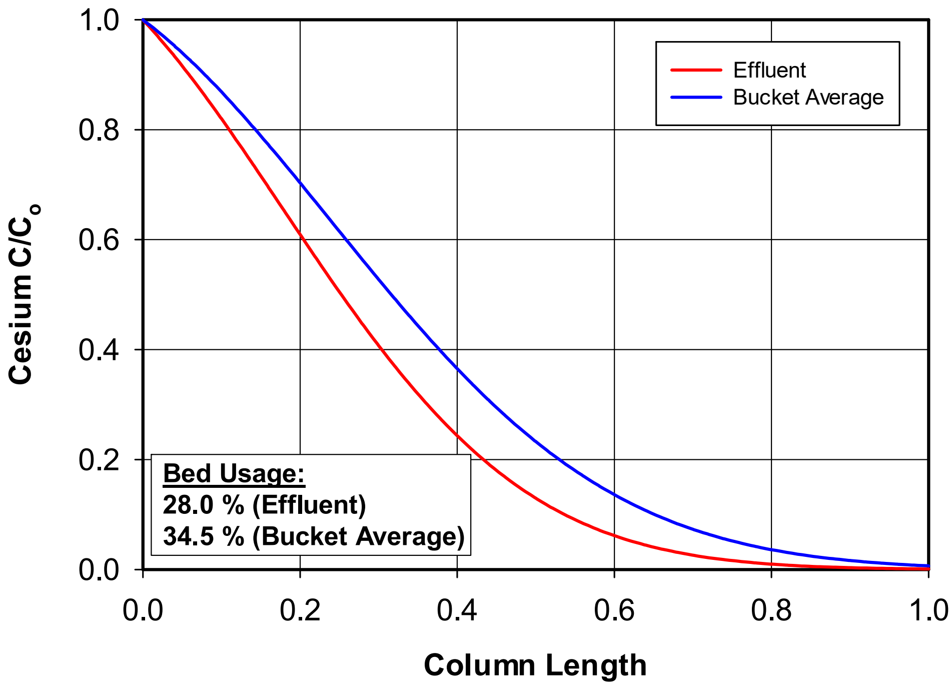

Figure A-6. Case 1c Column Concentration Profiles

Case 1d

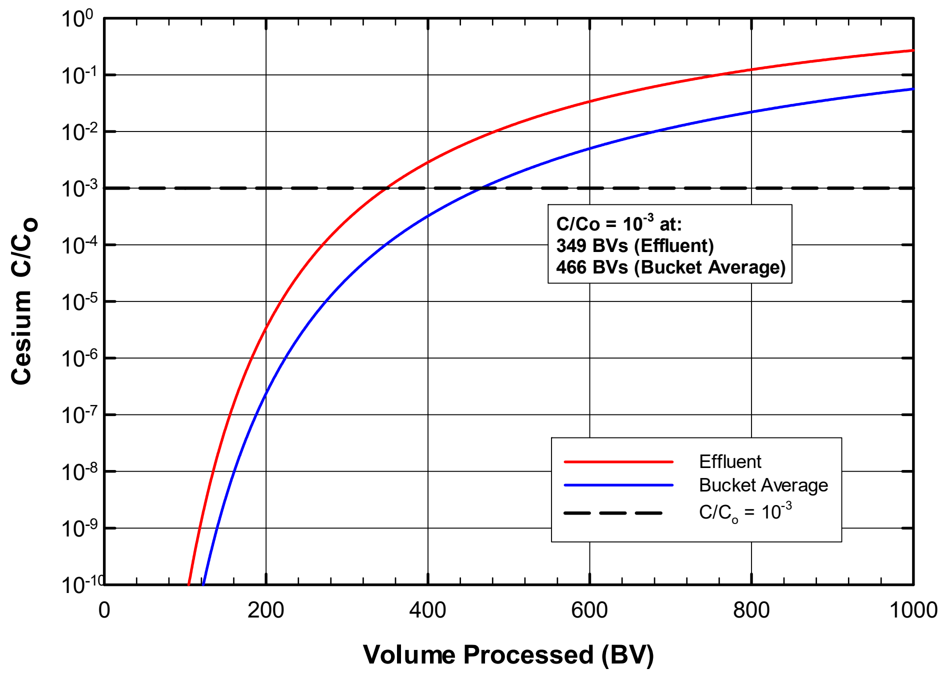

Figure A-7. Case 1d Breakthrough Curves

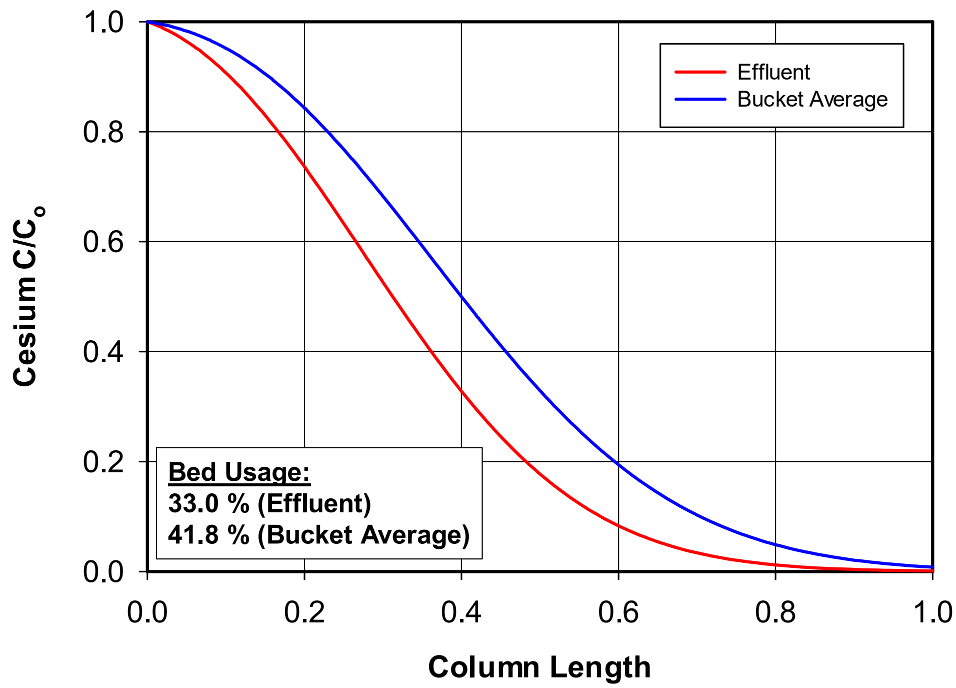

Figure A-8. Case 1d Column Concentration Profiles

Case 1e

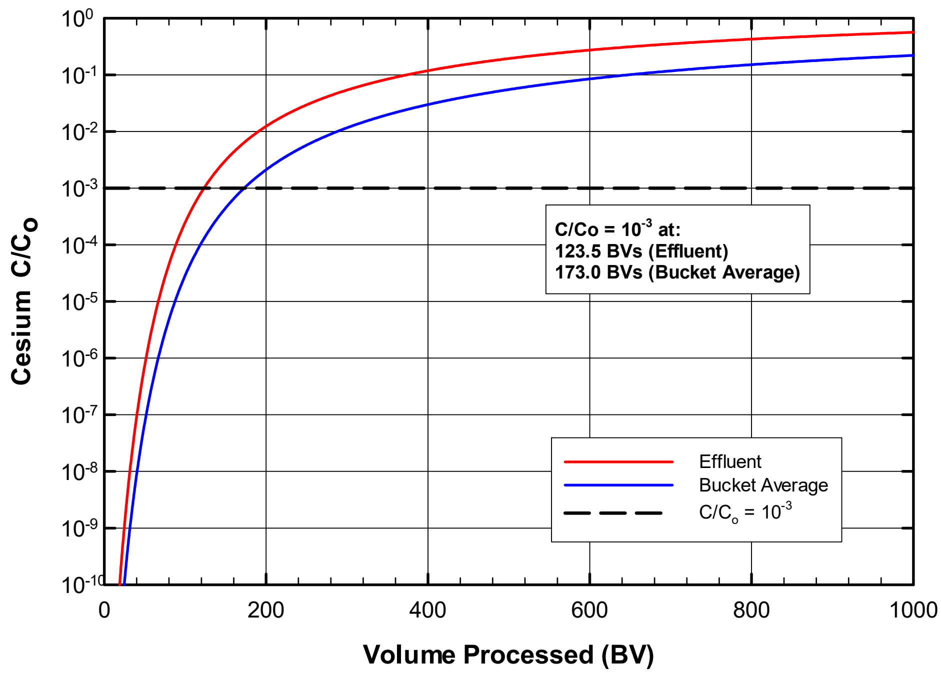

Figure A-9. Case 1e Breakthrough Curves

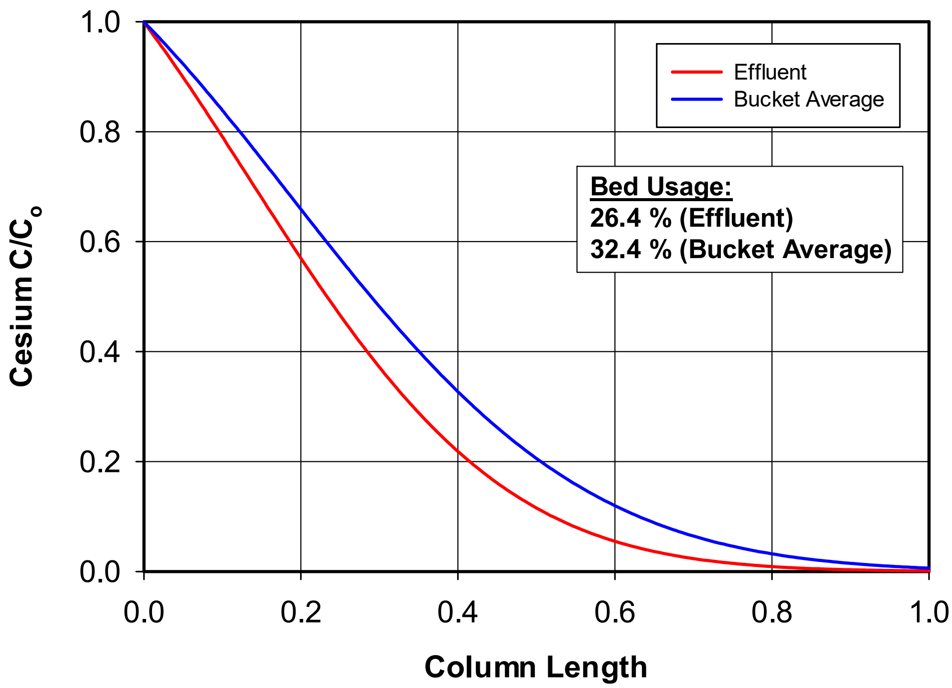

Figure A-10. Case 1e Column Concentration Profiles

Case 1f

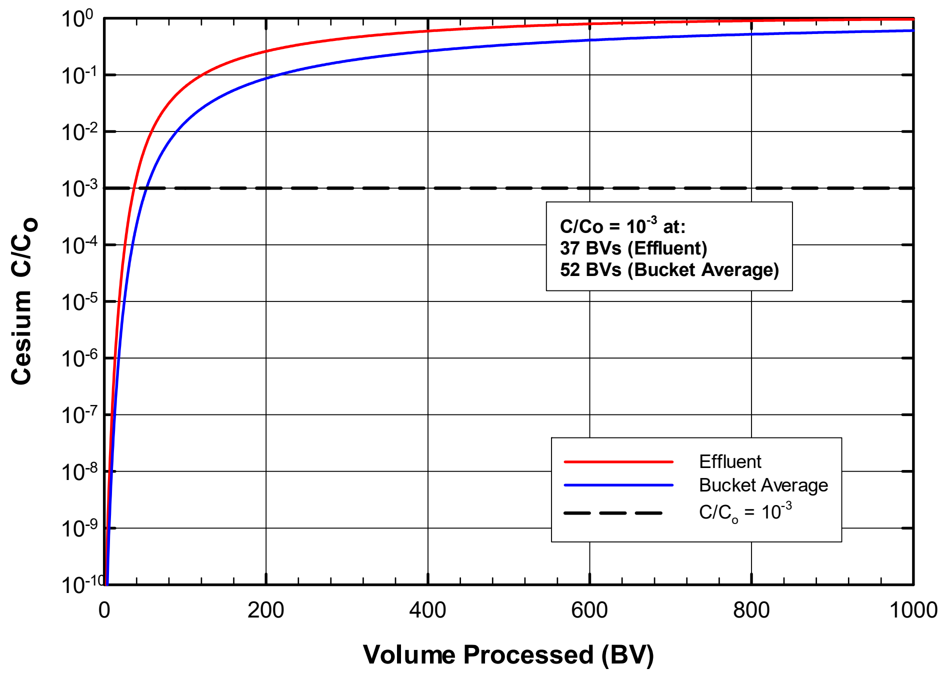

Figure A-11. Case 1f Breakthrough Curves

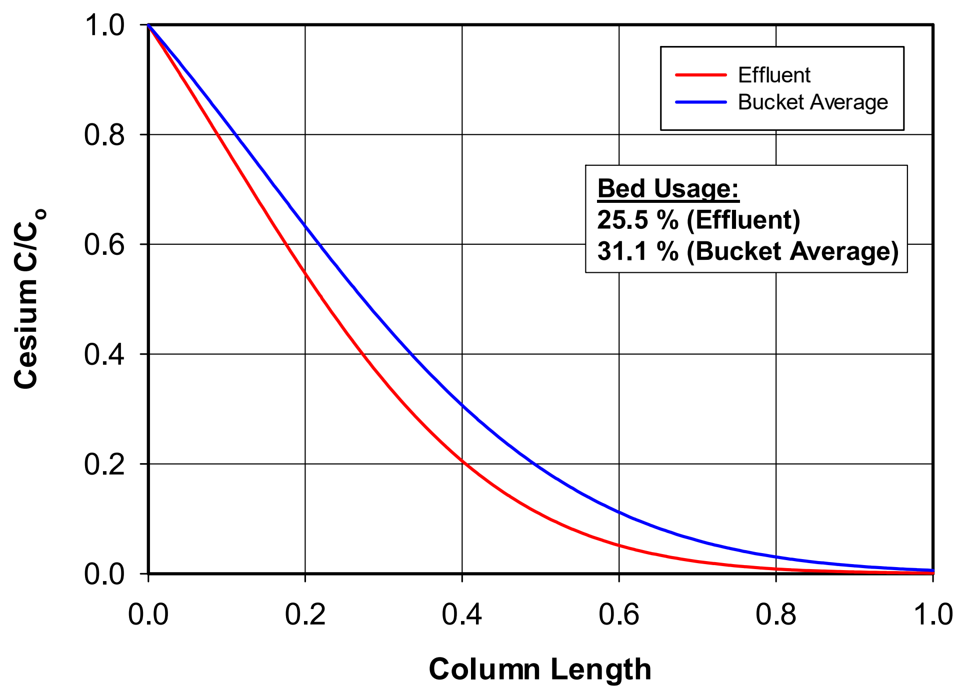

Figure A-12. Case 1f Column Concentration Profiles

Case 2a

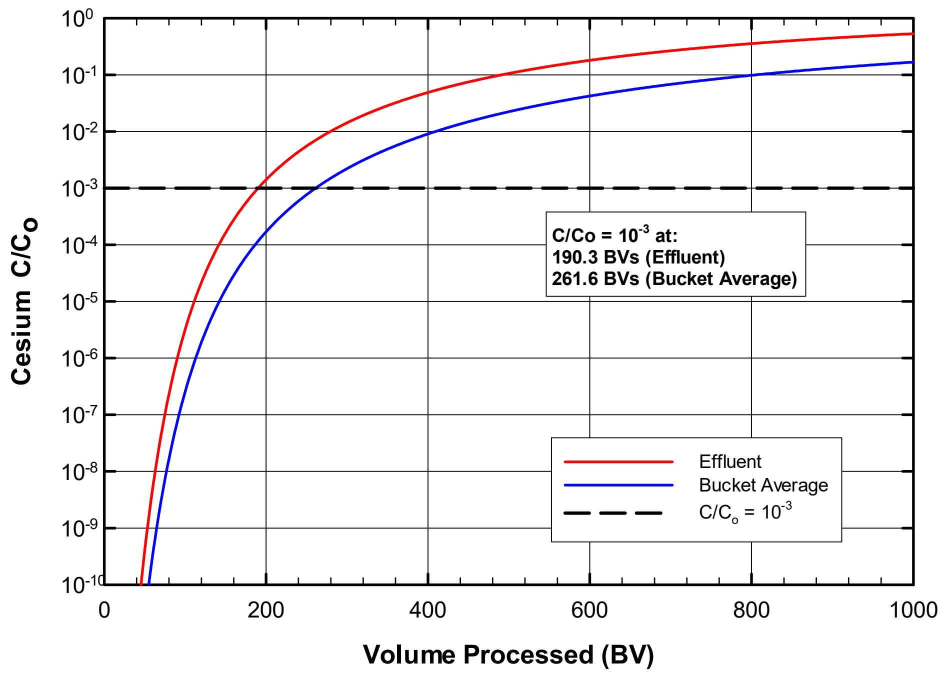

Figure A-13. Case 2a Breakthrough Curves

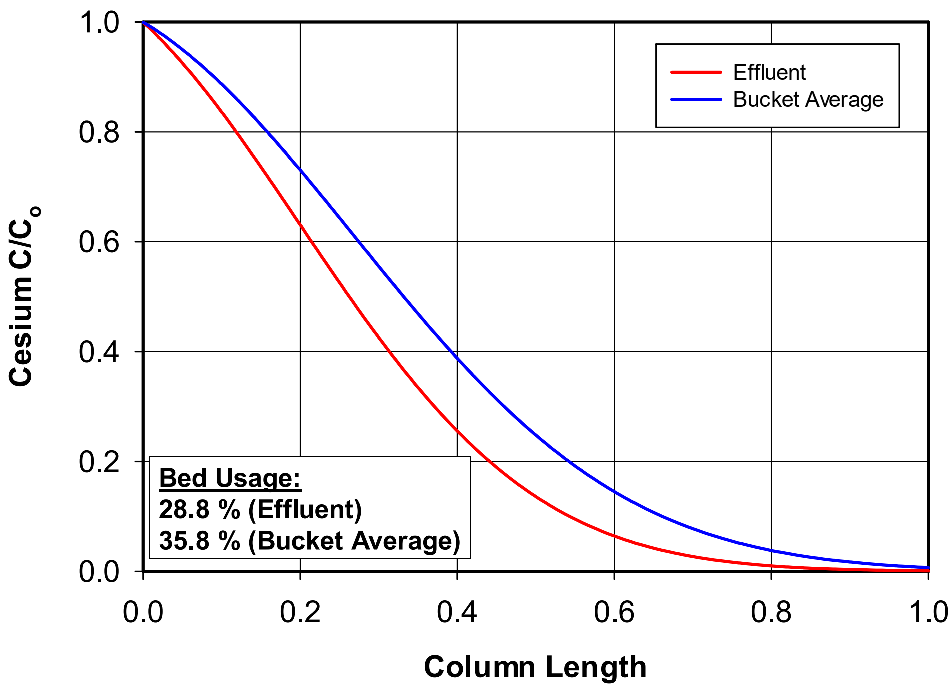

Figure A-14. Case 2a Column Concentration Profiles

Case 2b

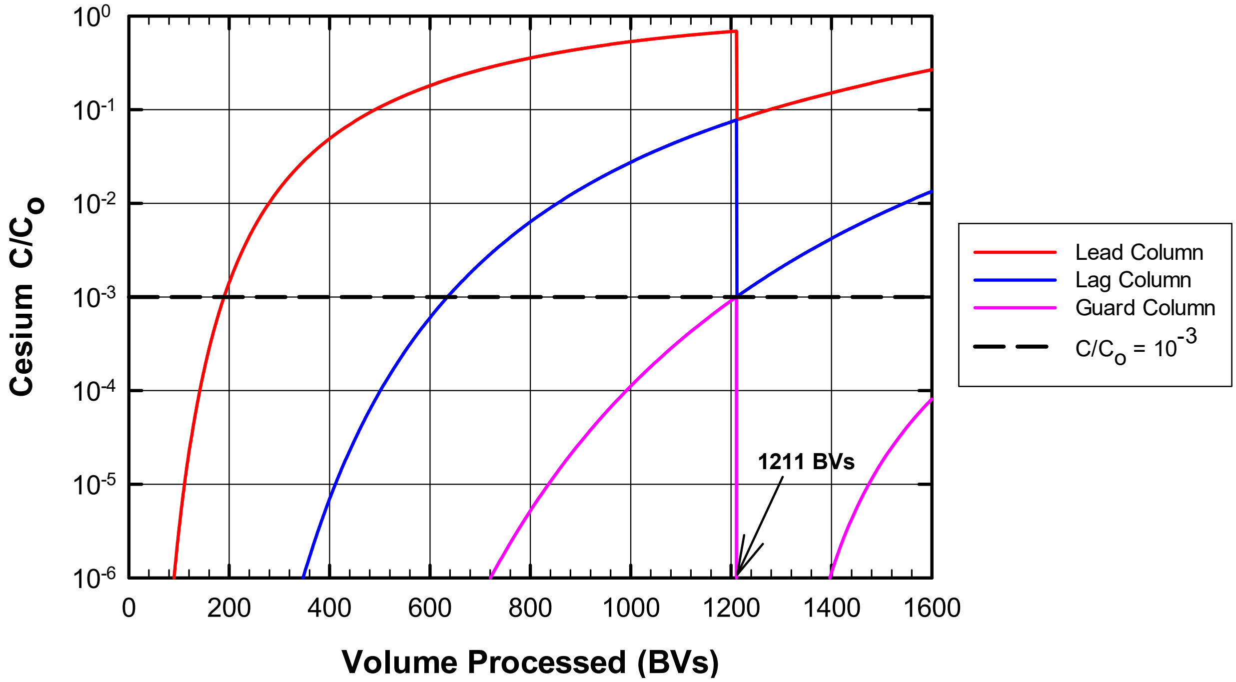

Figure A-15. Case 2b Breakthrough Curves

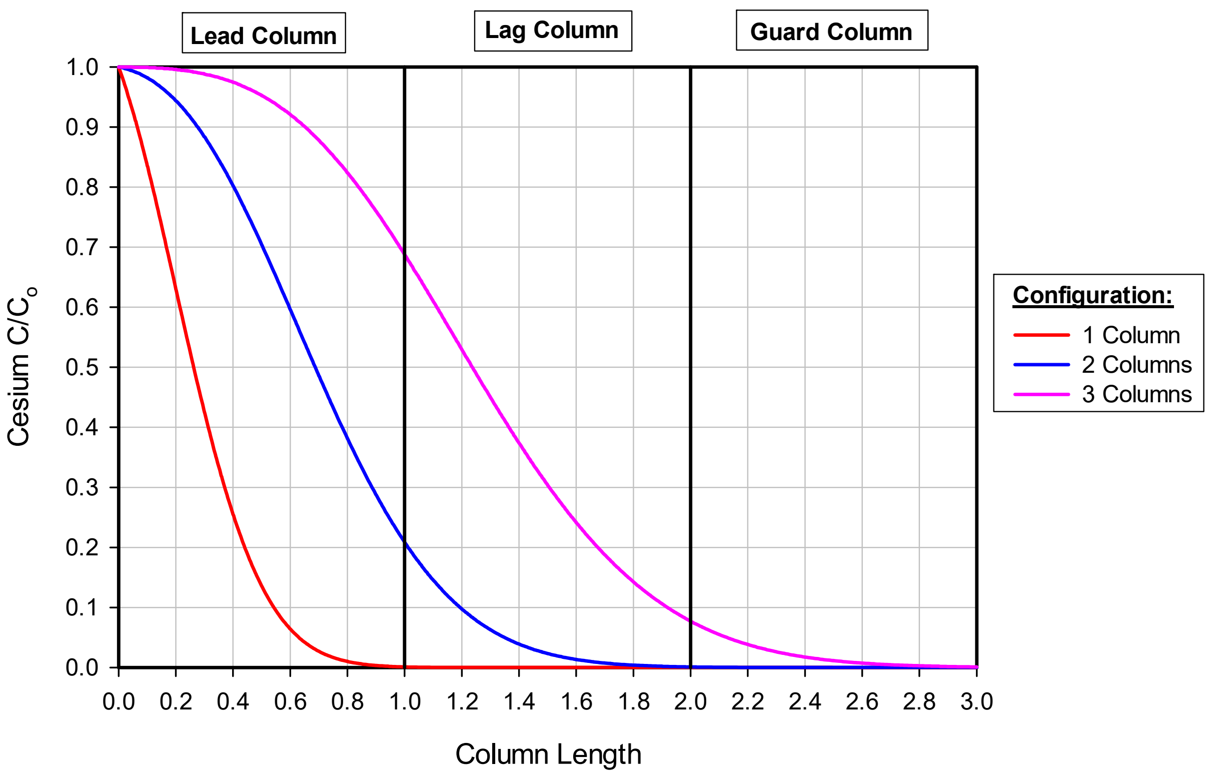

Figure A-16. Case 2b Column Concentration Profiles

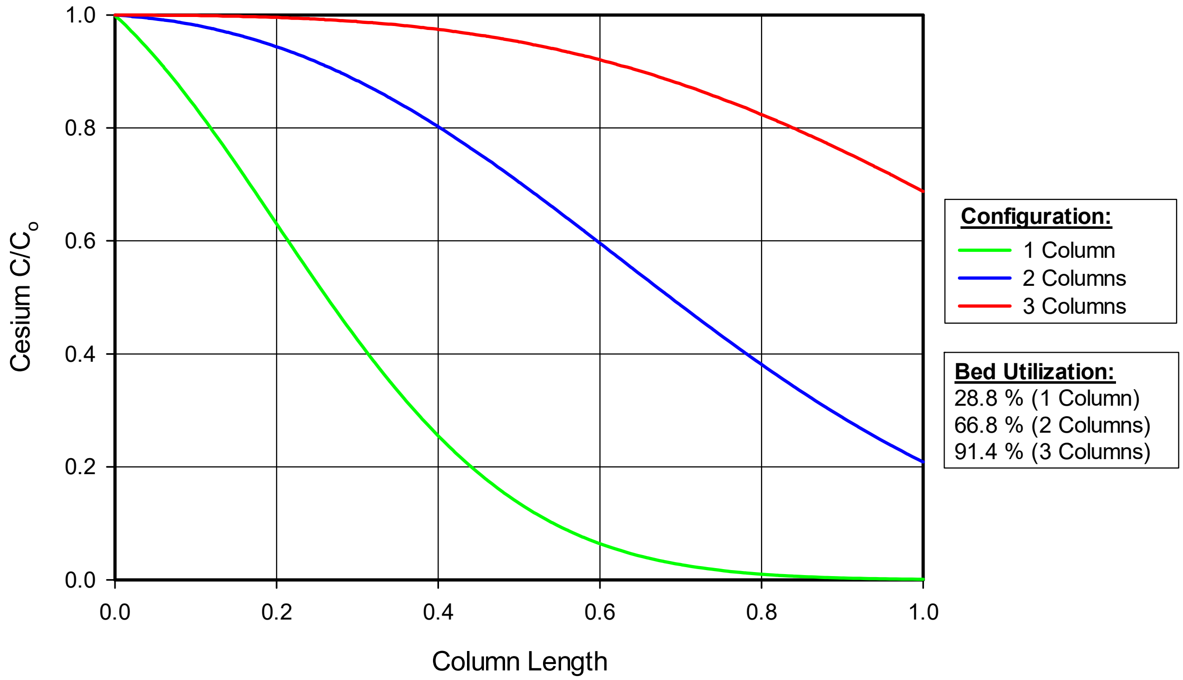

Figure A-17. Case 2b Lead Column Concentration Profiles

Case 2c

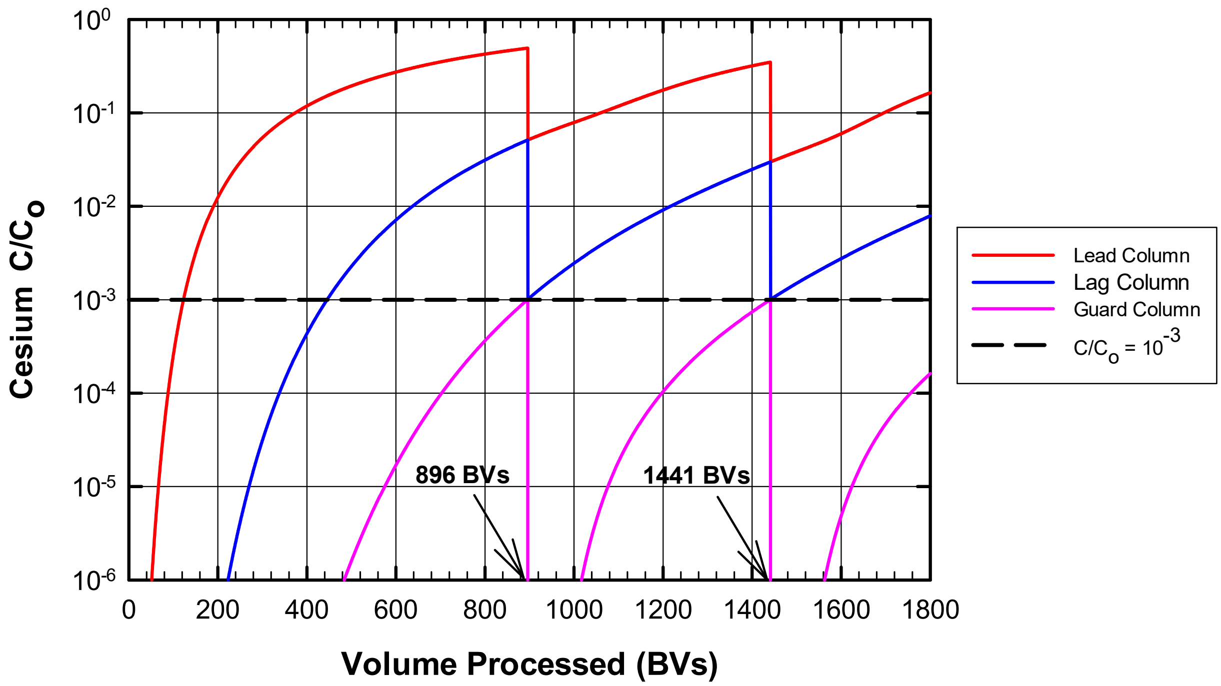

Figure A-18. Case 2c Breakthrough Curves

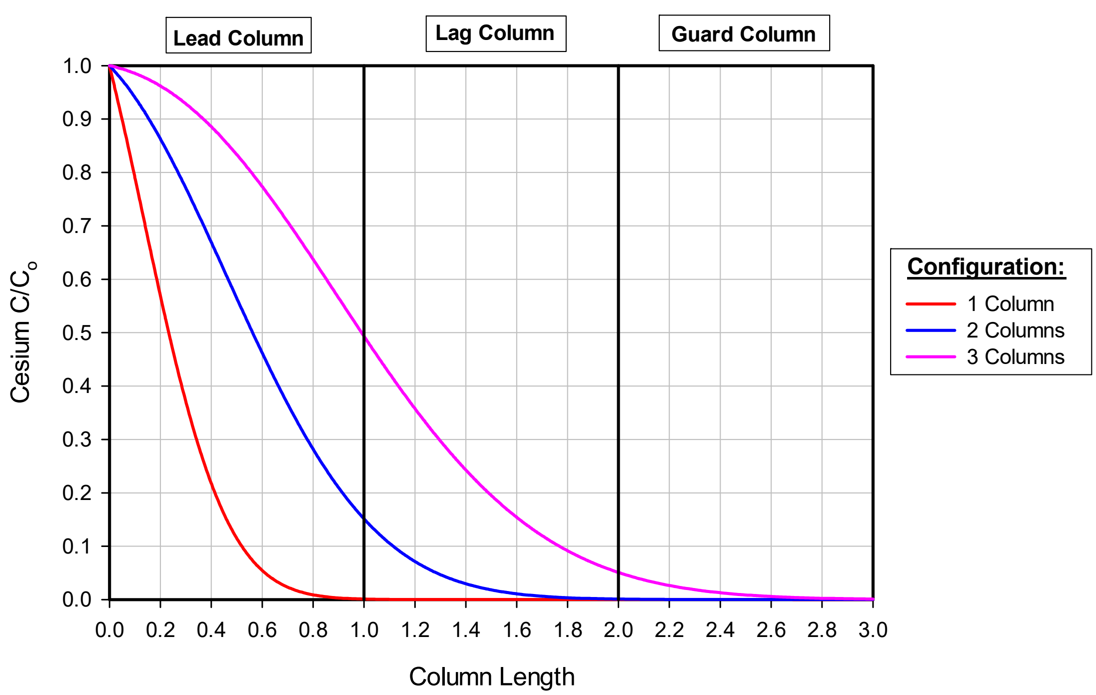

Figure A-19. Case 2c Column Concentration Profiles

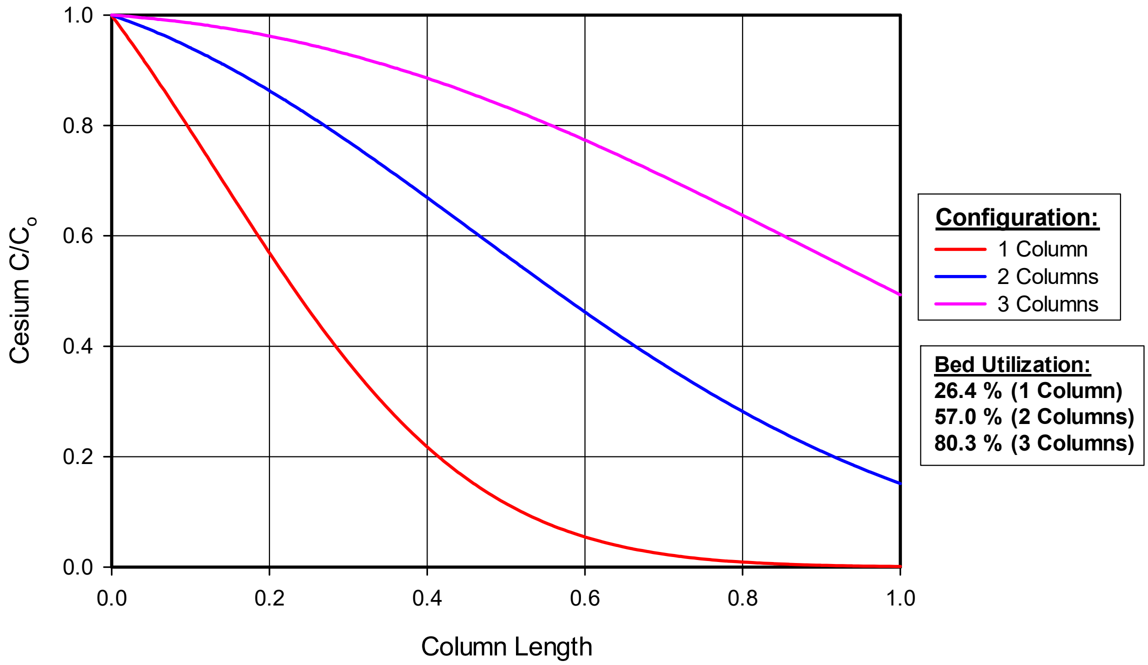

Figure A-20. Case 2c Lead Column Concentration Profiles

Case 2d

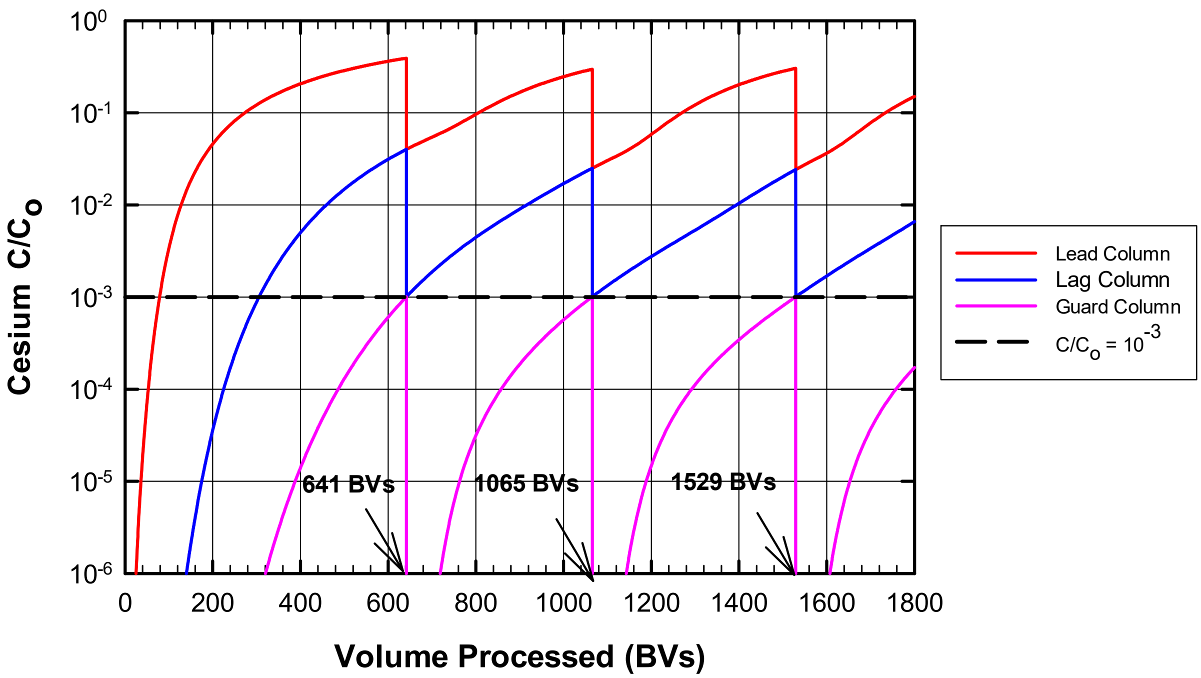

Figure A-21. Case 2d Breakthrough Curves

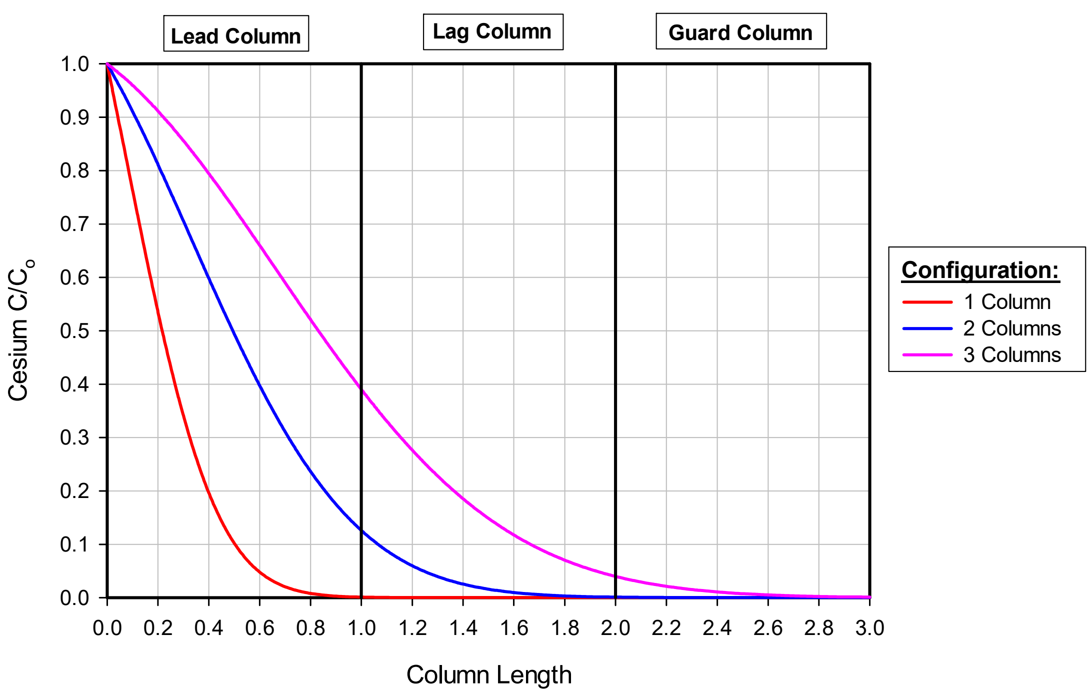

Figure A-22. Case 2d Column Concentration Profiles

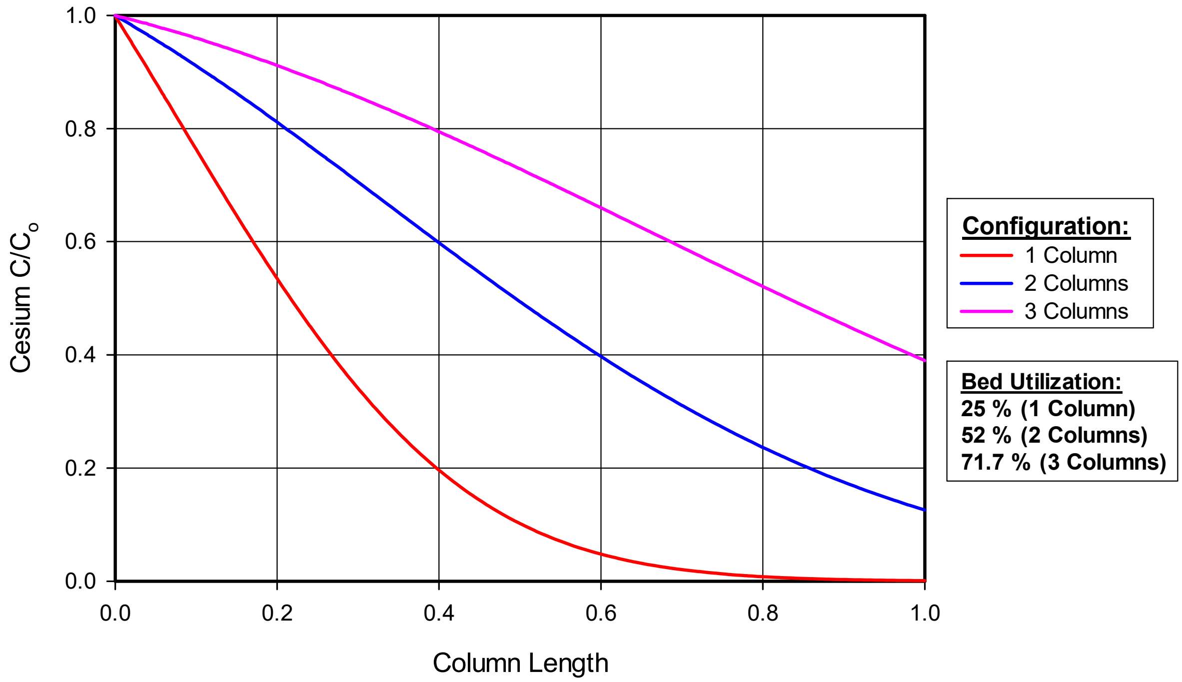

Figure A-23. Case 2d Lead Column Concentration Profiles

Case 2e

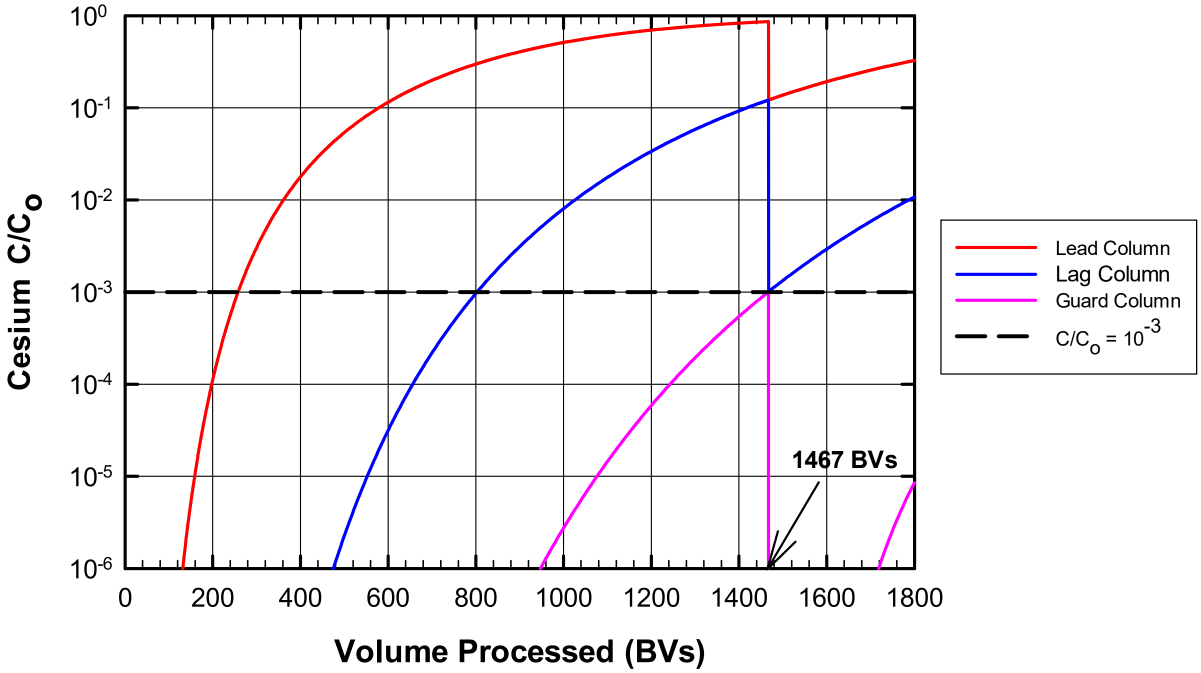

Figure A-24. Case 2e Breakthrough Curves

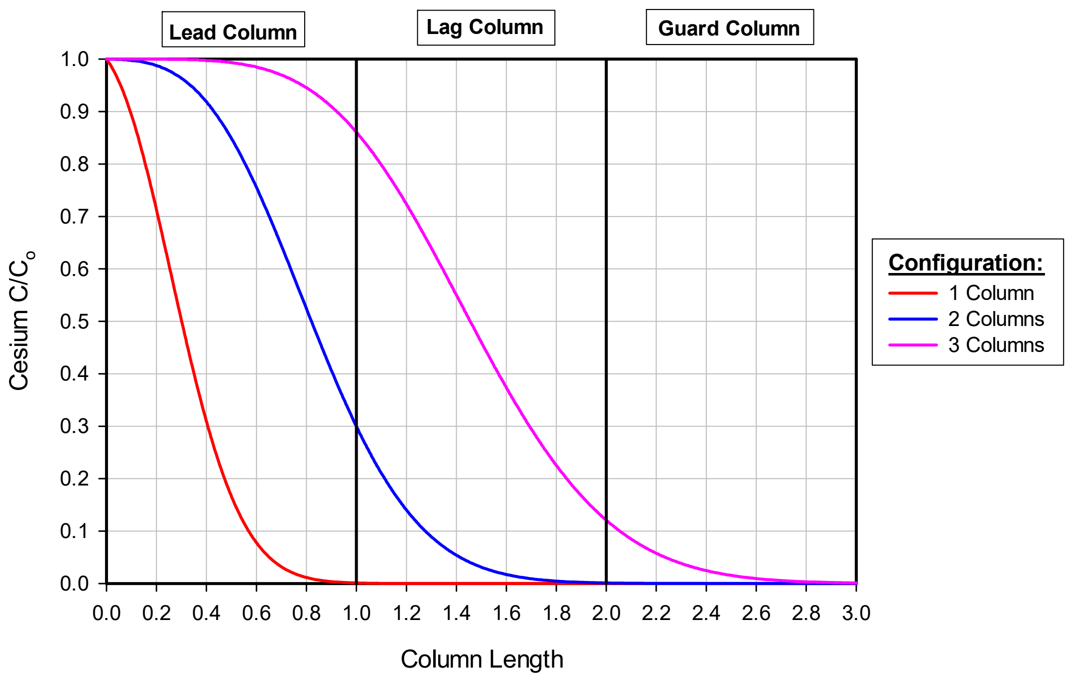

Figure A-25. Case 2e Column Concentration Profiles

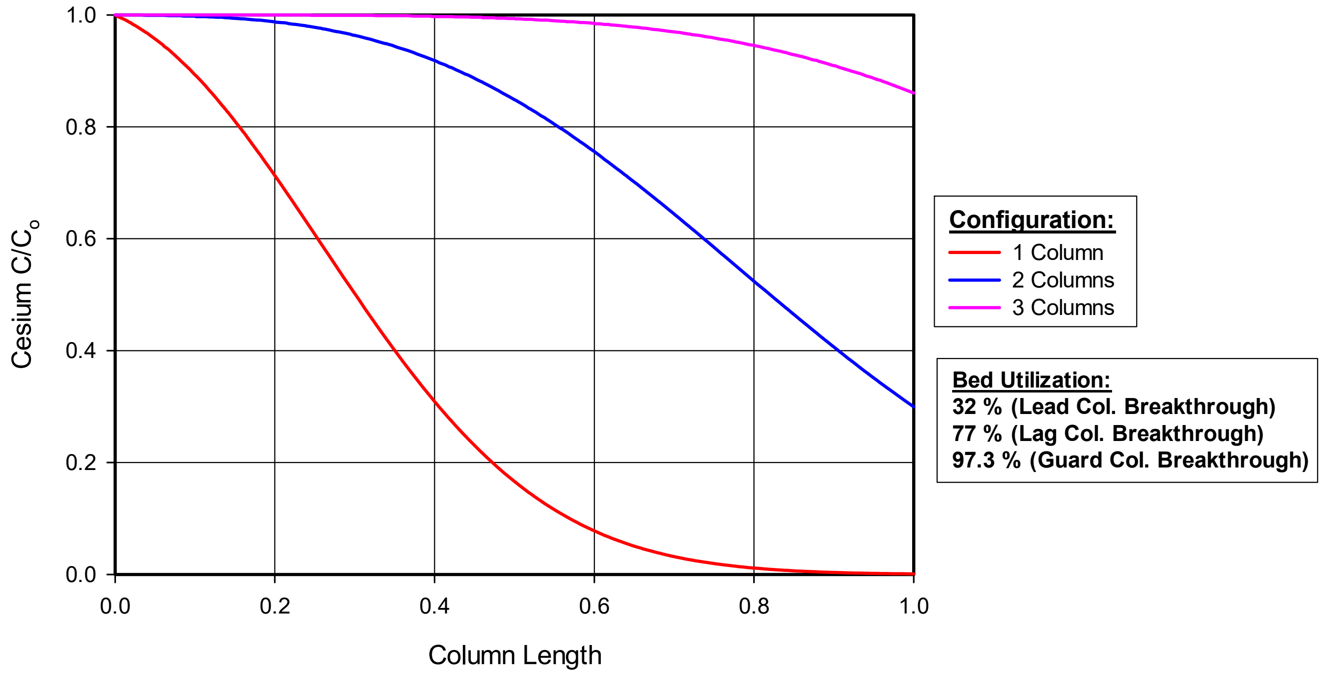

Figure A-26. Case 2e Lead Column Concentration Profiles

<u>Case 2ee</u>
(Note: Case 2ee has the same configuration as Case 2e but using parameters recommended by L. L. Hamm)

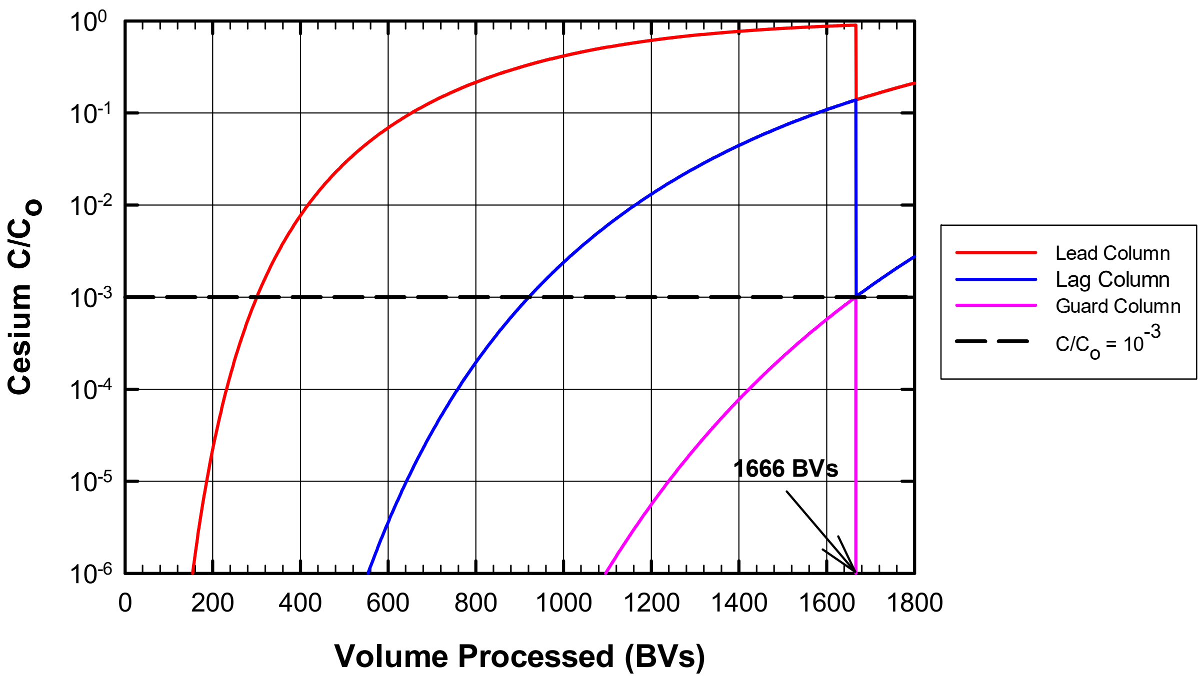

Figure A-27. Case 2ee Breakthrough Curves

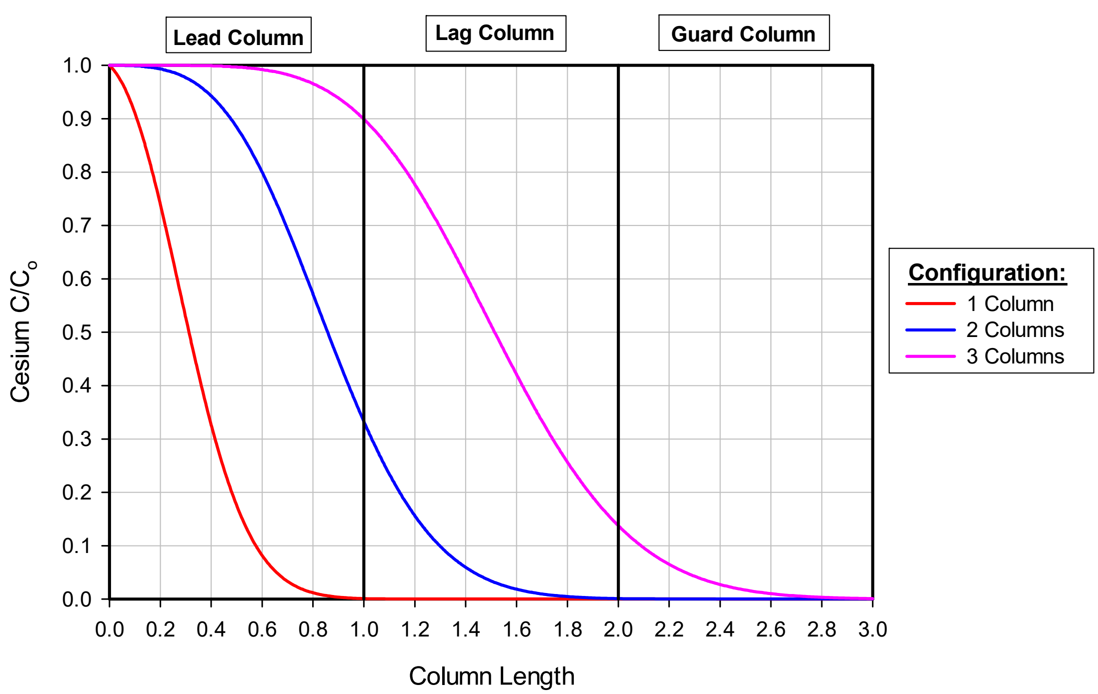

Figure A-28. Case 2ee Column Concentration Profiles

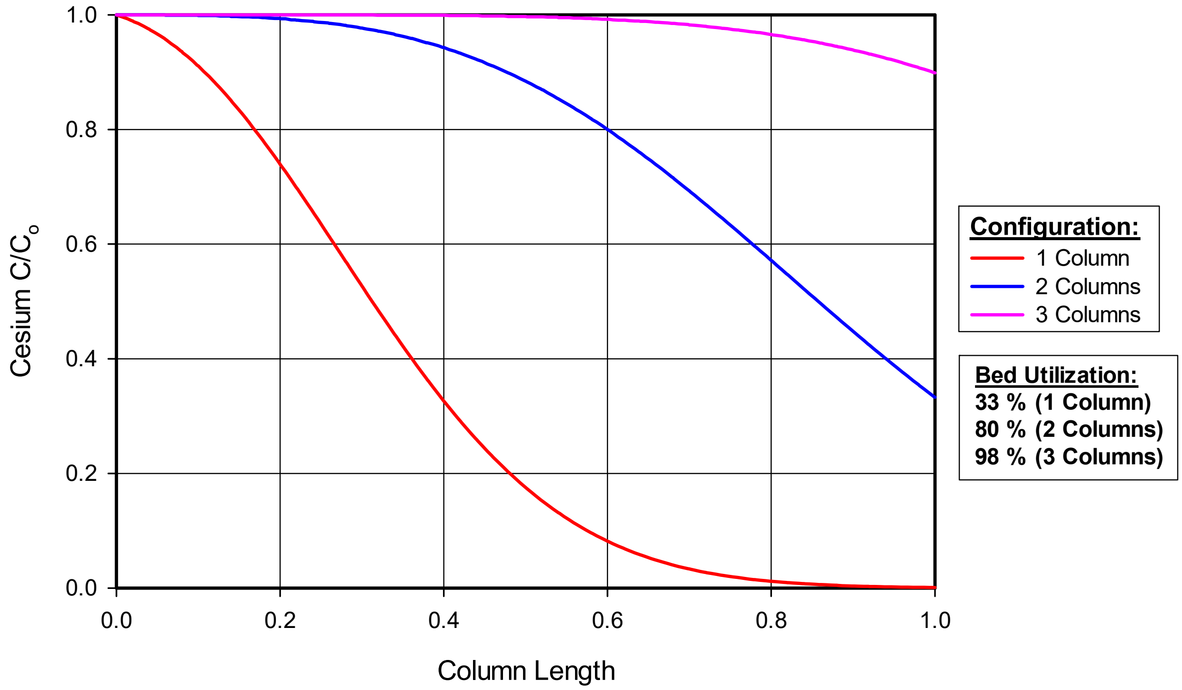

Figure A-29. Case 2ee Lead Column Concentration Profiles

Case 2f

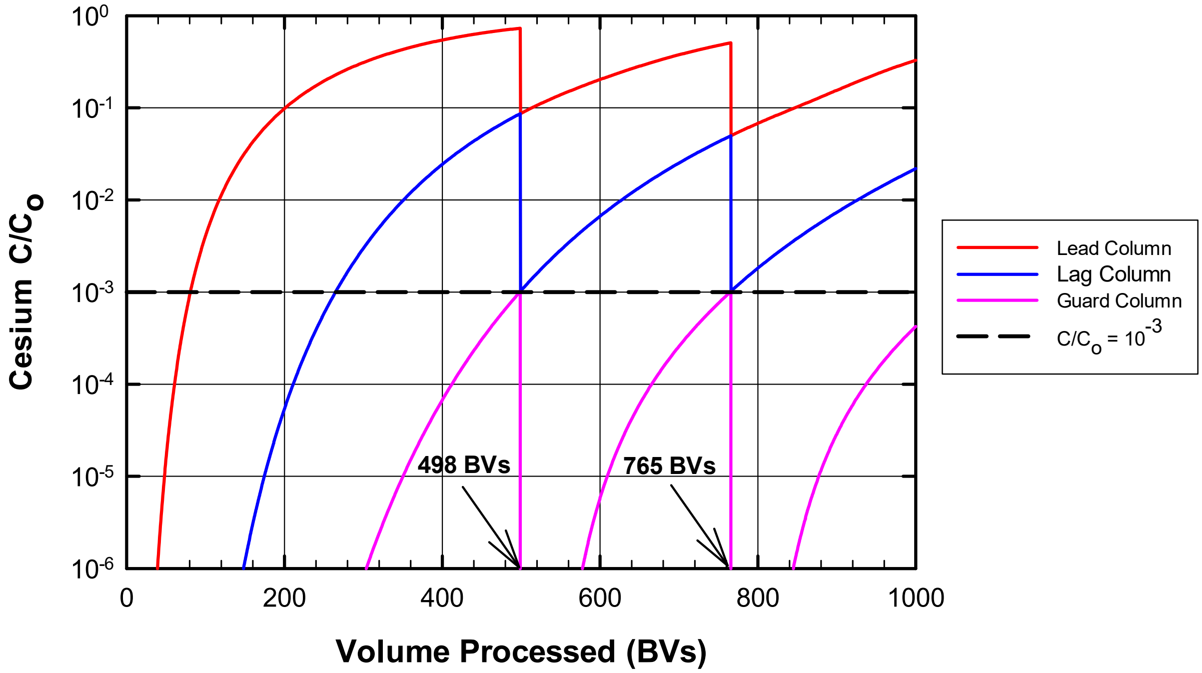

Figure A-30. Case 2f Breakthrough Curves

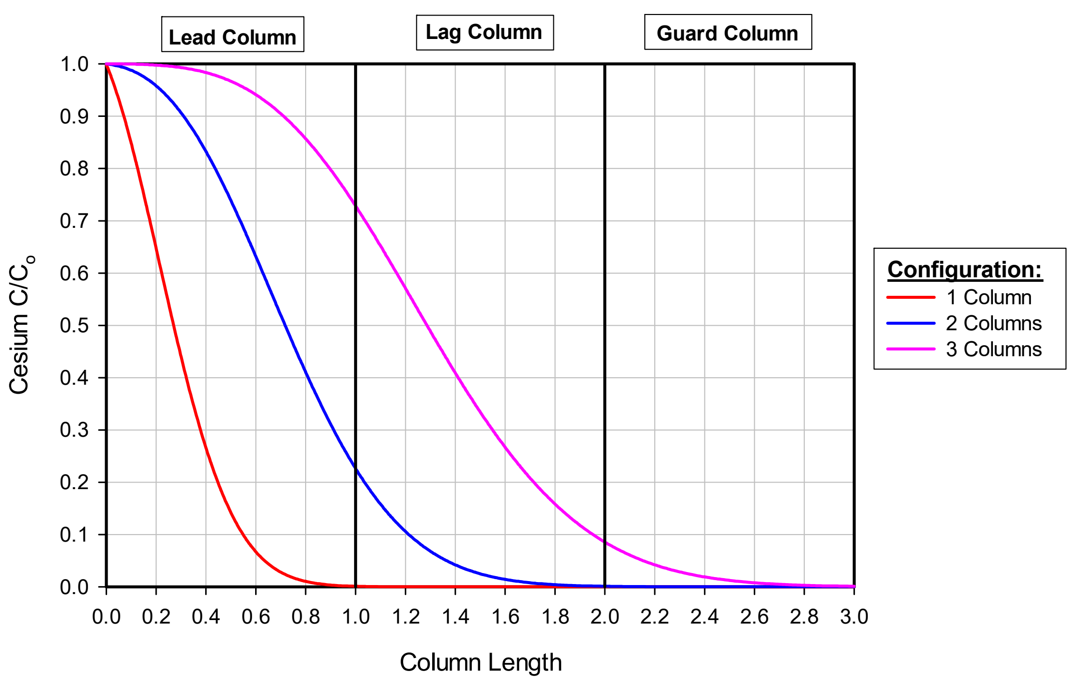

Figure A-31. Case 2f Column Concentration Profiles

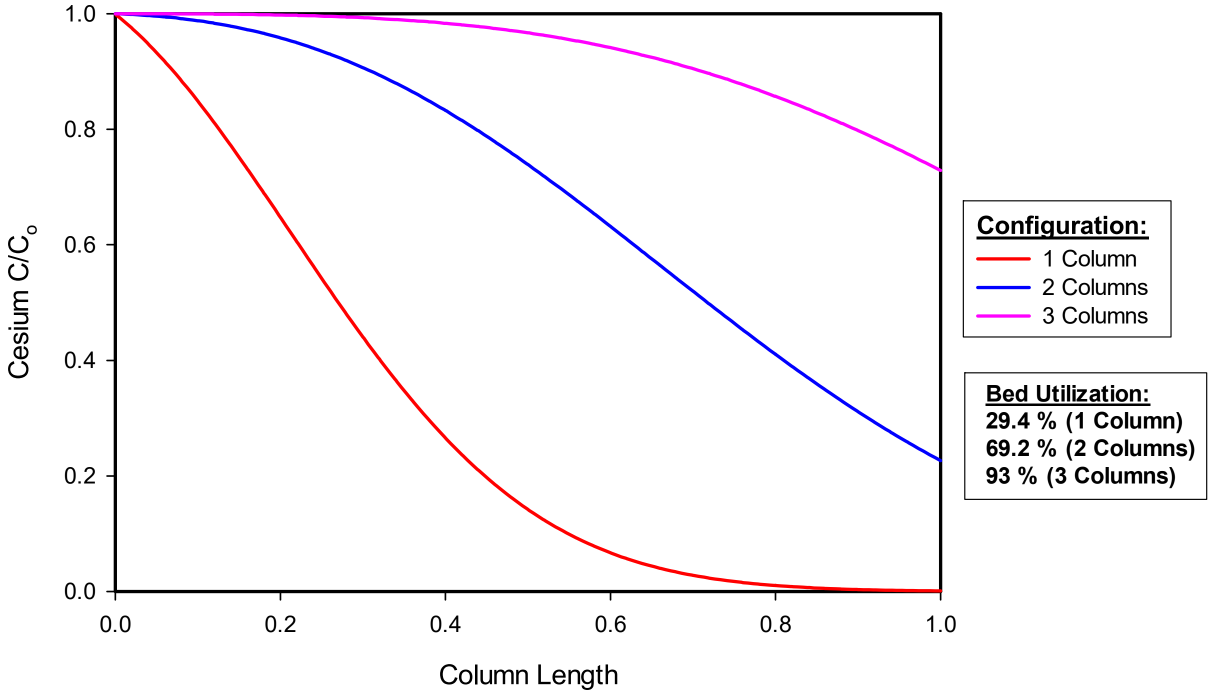

Figure A-32. Case 2f Lead Column Concentration Profiles

Case 2ff
(Note: Case 2ff has the same configuration as Case 2f but using parameters recommended by L. L. Hamm)

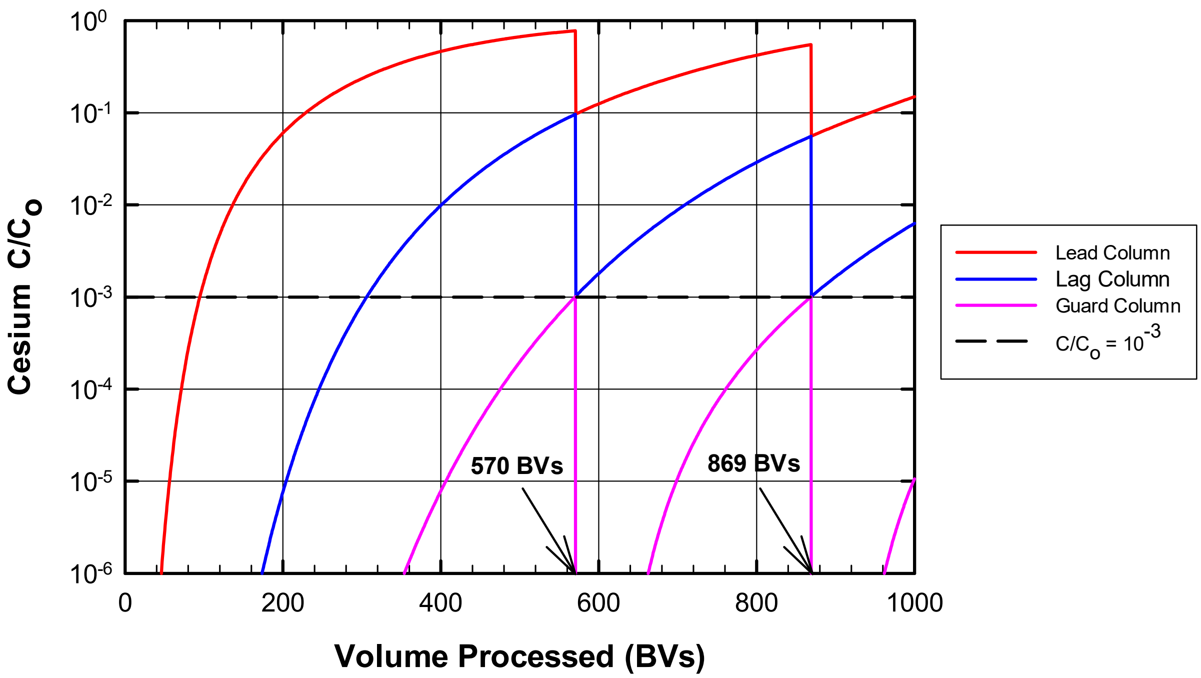

Figure A-33. Case 2ff Breakthrough Curves

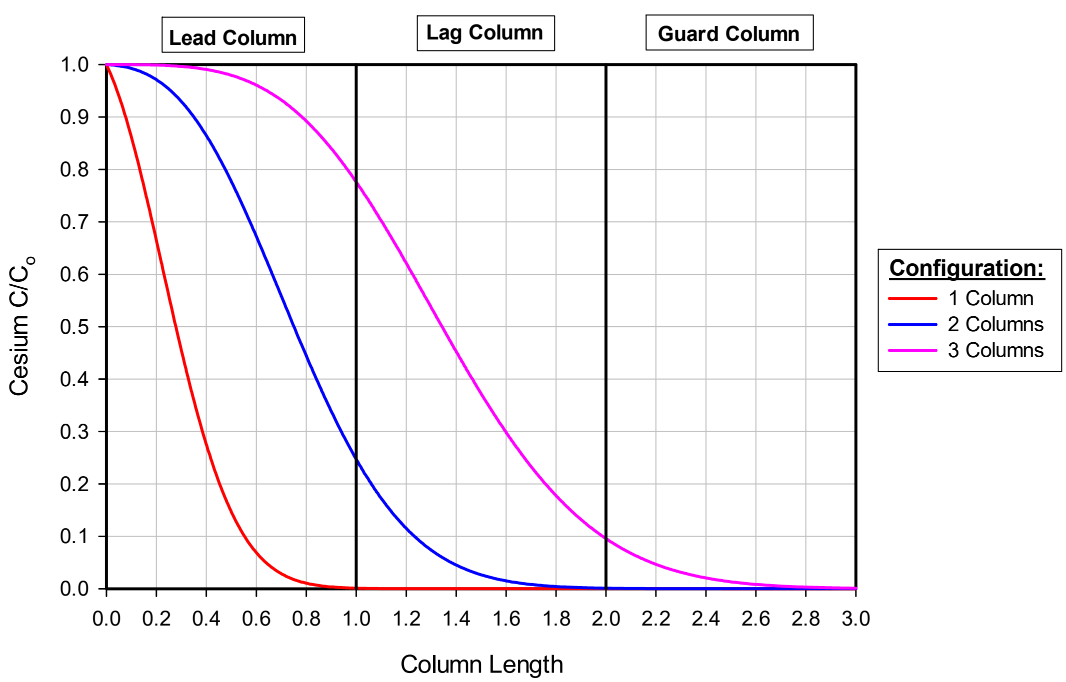

Figure A-34. Case 2ff Column Concentration Profiles

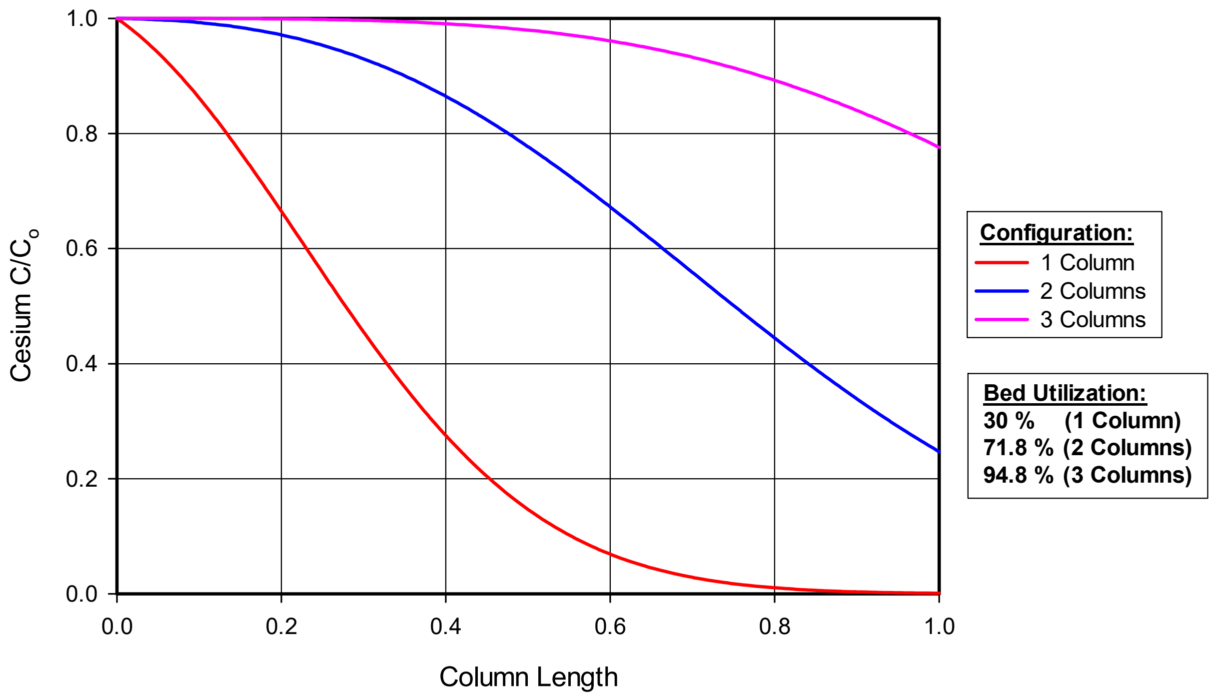

Figure A-35. Case 2ff Lead Column Concentration Profiles

Case 2g

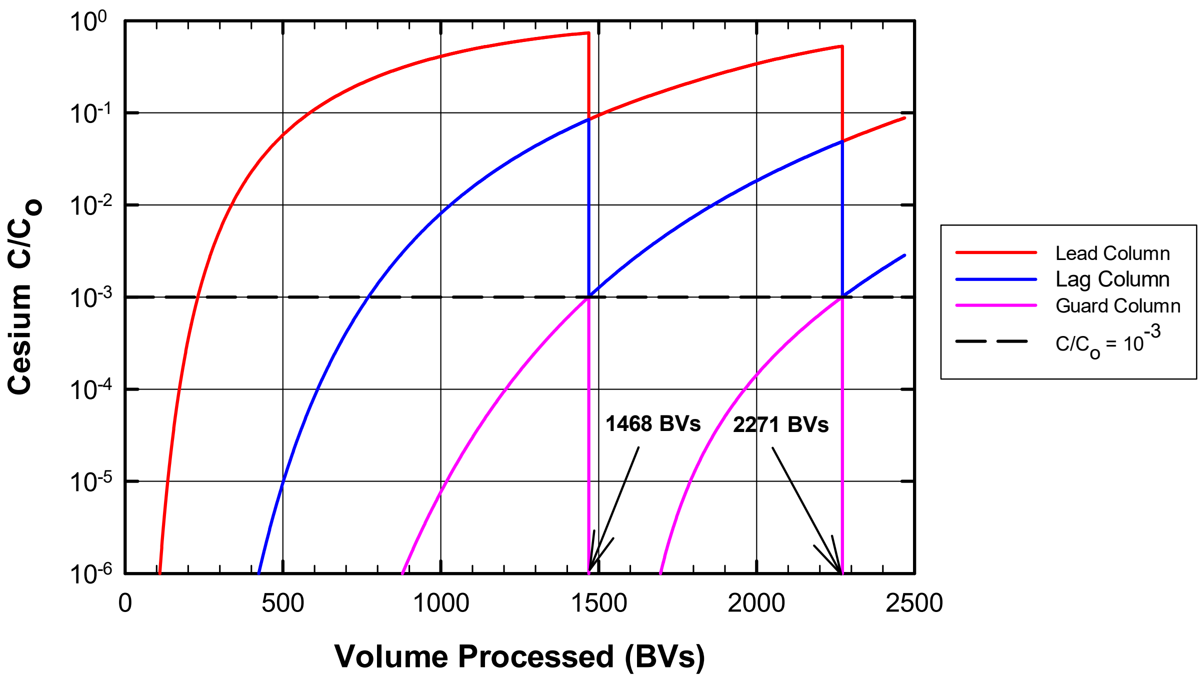

Figure A-36. Case 2g Breakthrough Curves

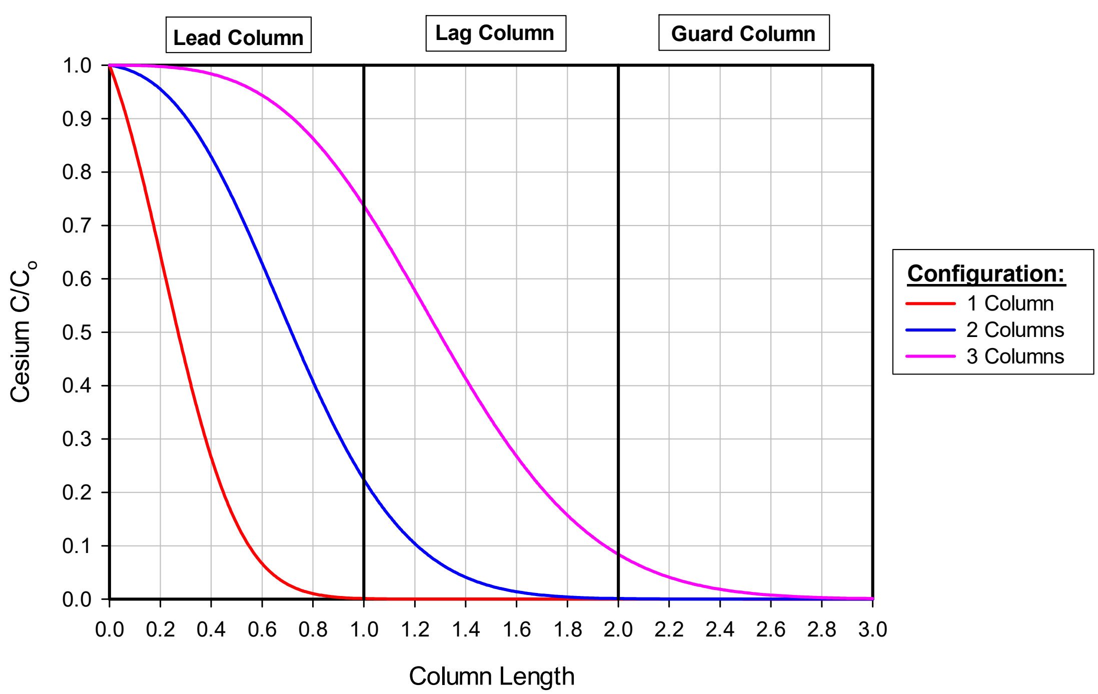

Figure A-37. Case 2g Column Concentration Profiles

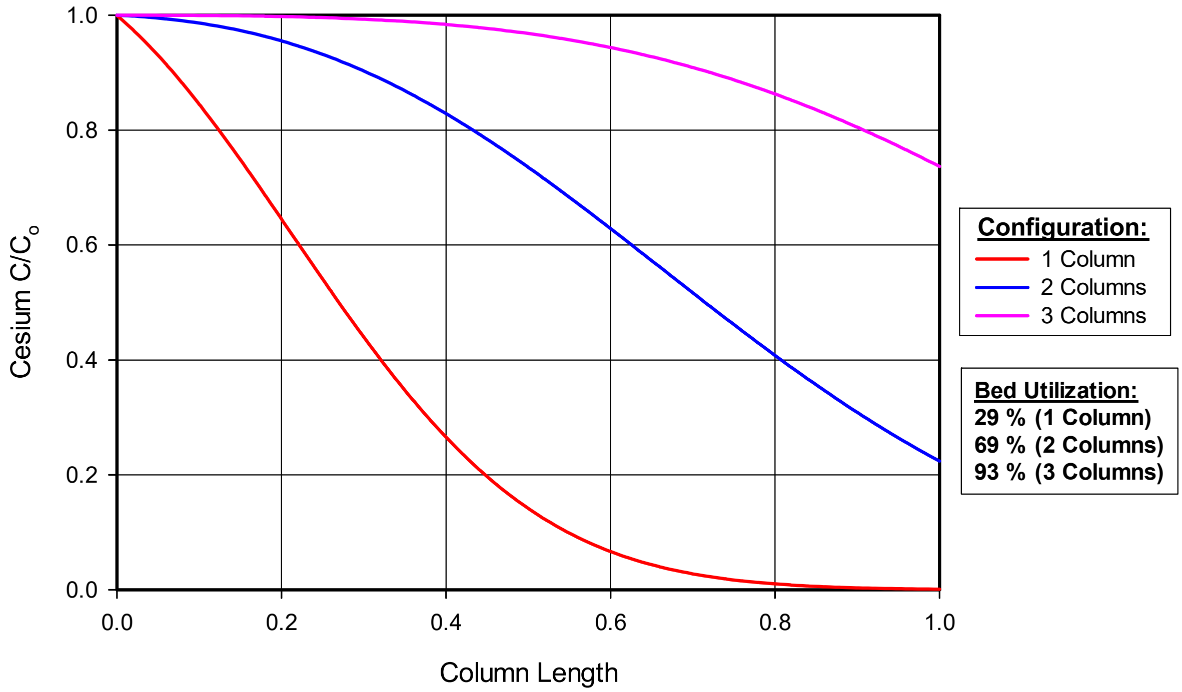

Figure A-38. Case 2g Lead Column Concentration Profiles

Case 3a

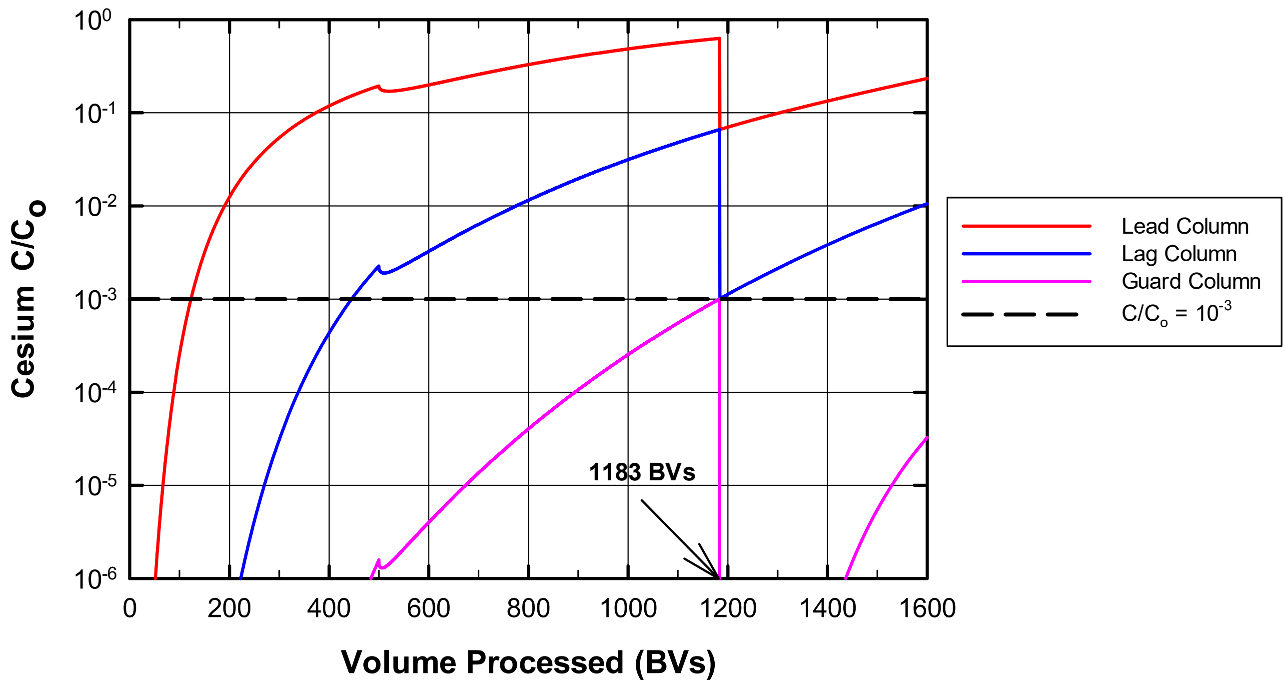

Figure A-39. Case 3a Breakthrough Curves

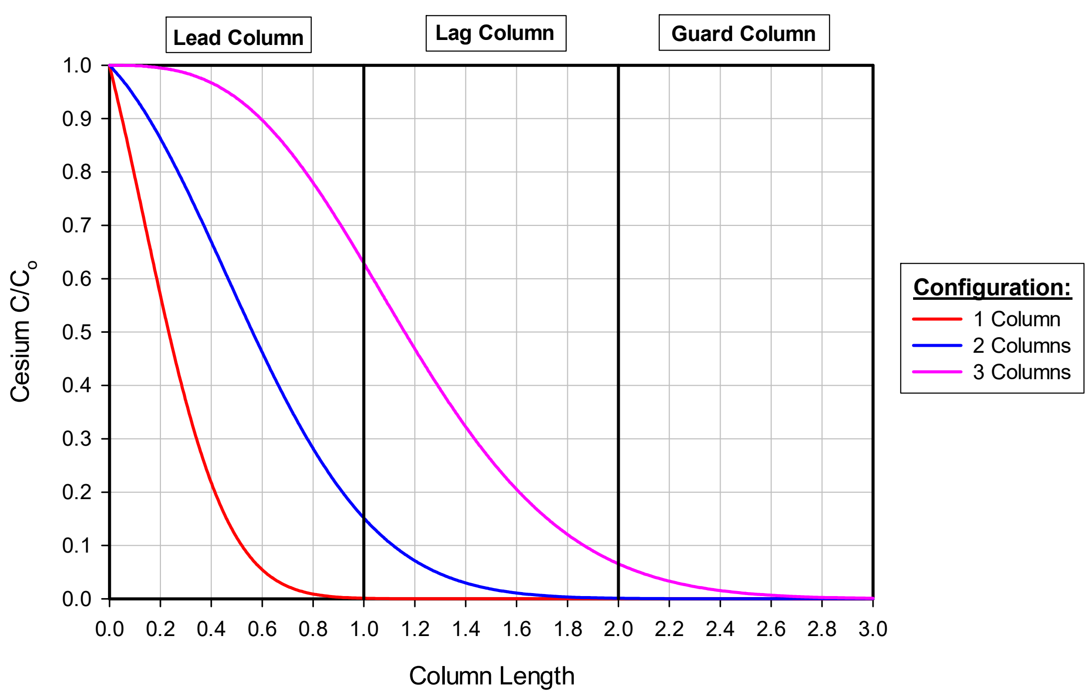

Figure A-40. Case 3a Column Concentration Profiles

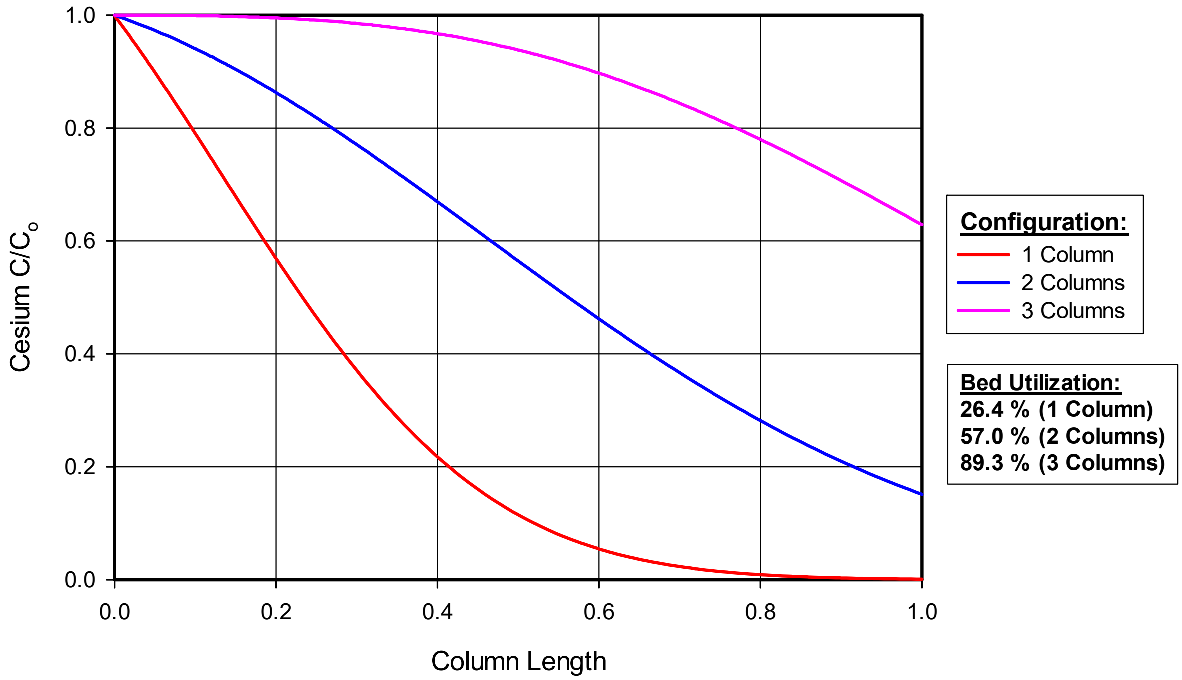

Figure A-41. Case 3a Lead Column Concentration Profiles

Case 5a

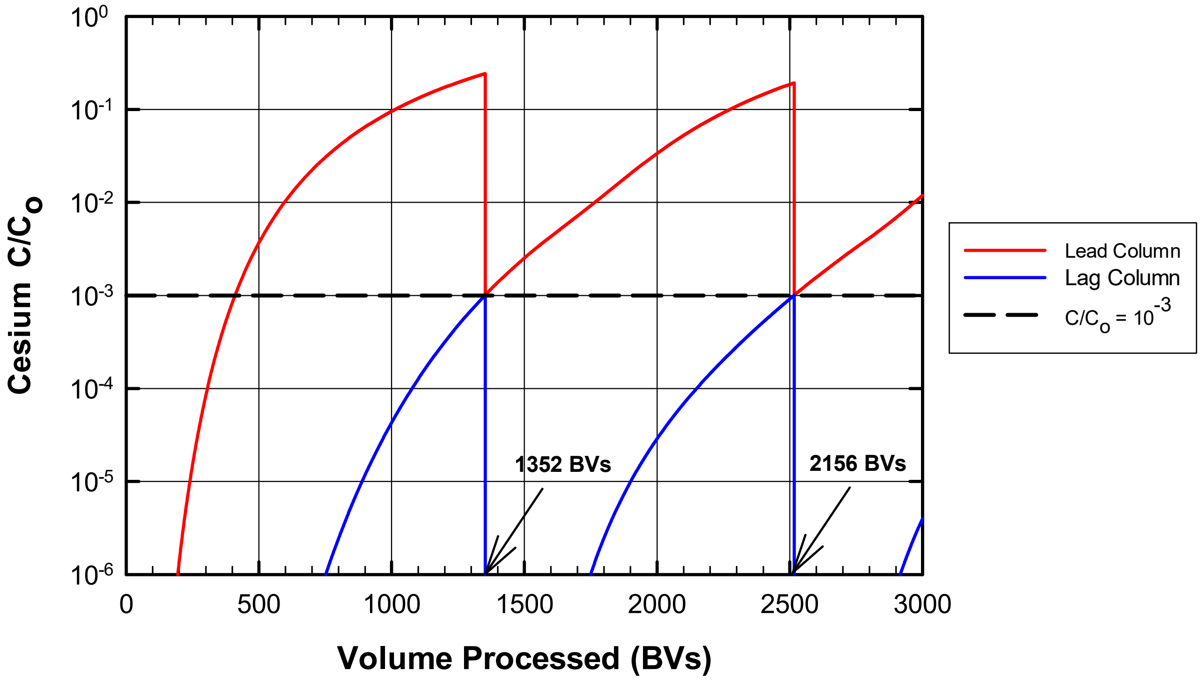

Figure A-42. Case 5a Breakthrough Curves based on Effluent Concentrations

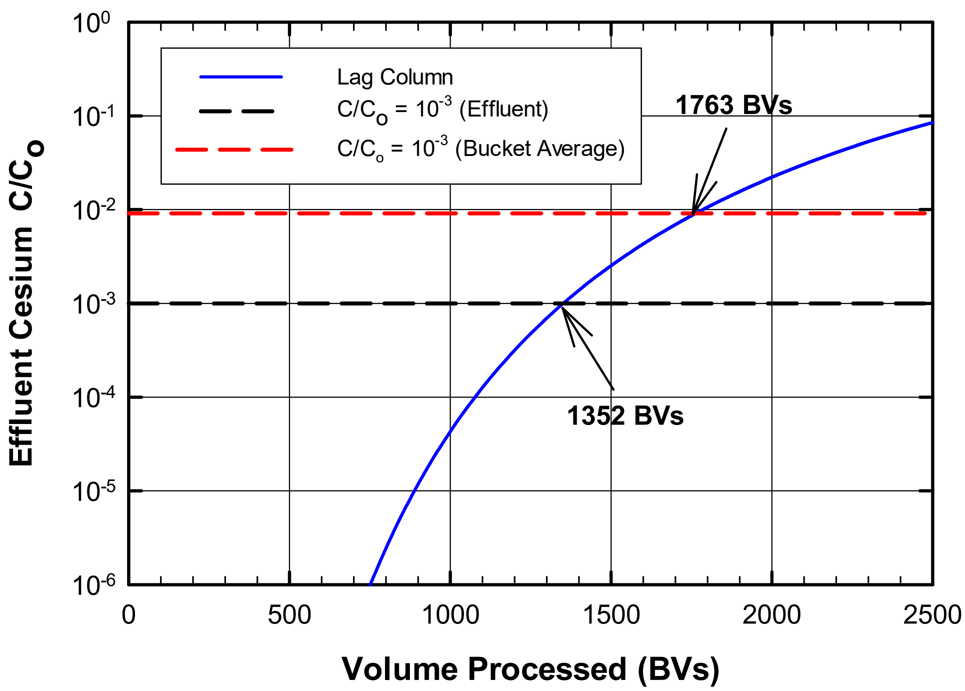

Figure A-43. Case 5a Breakthrough based on Effluent and Bucket-Average Concentrations

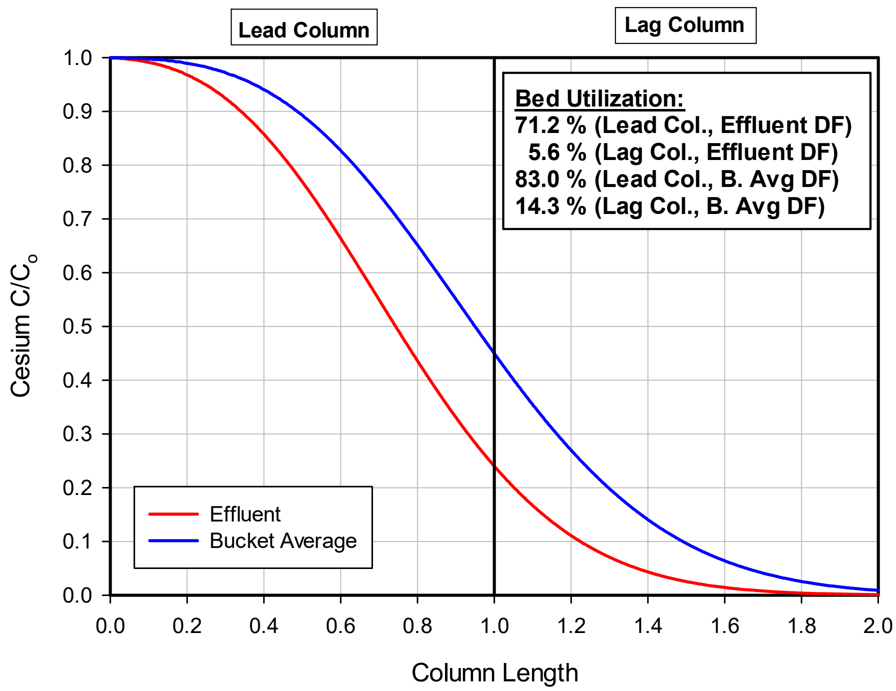

Figure A-44. Case 5a Column Concentration Profiles

Case 5b

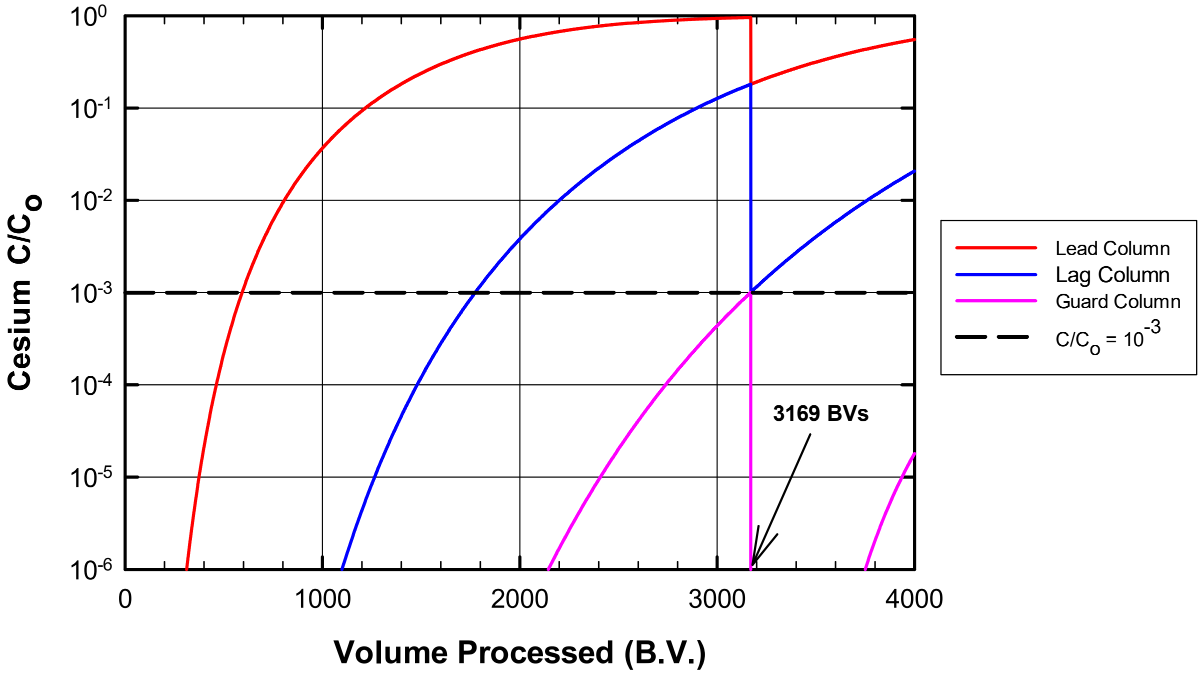

Figure A-45. Case 5b Breakthrough Curves based on Effluent Concentrations

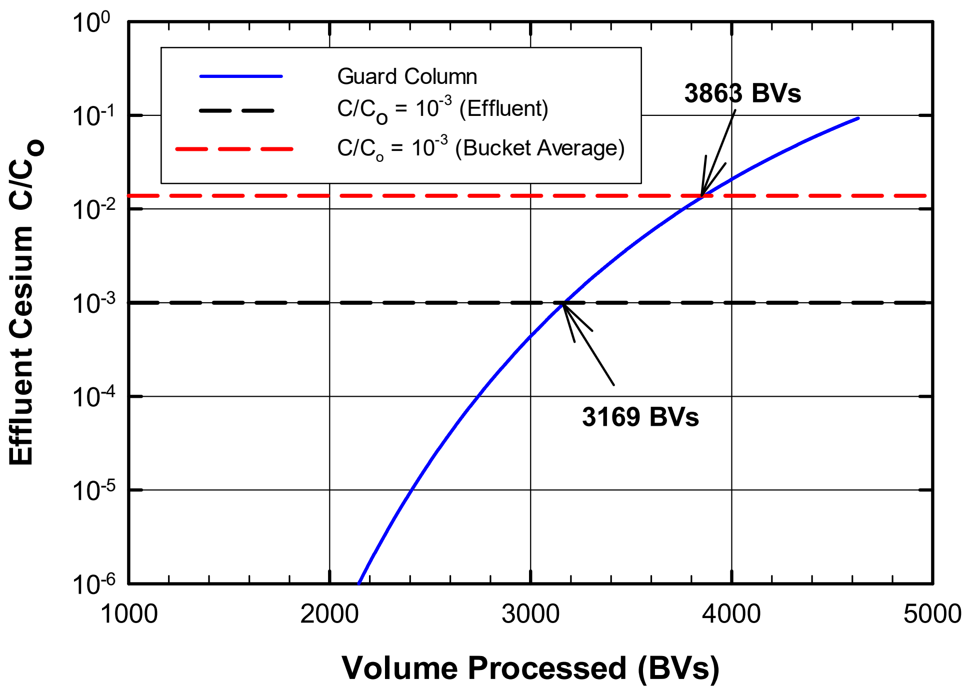

Figure A-46. Case 5b Breakthrough based on Effluent and Bucket-Average Concentrations

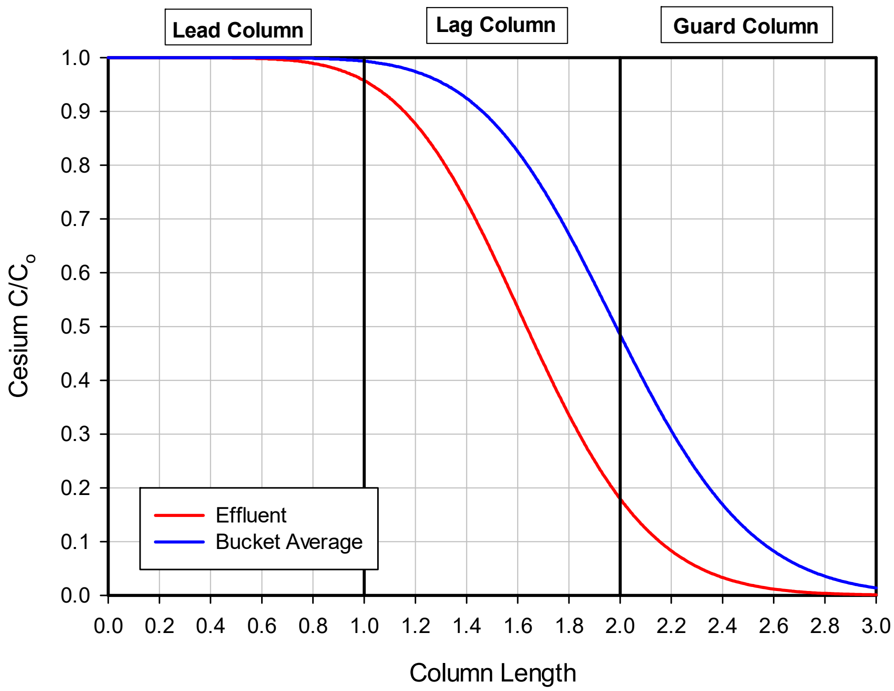

Figure A-47. Case 5b Column Concentration Profiles

Case 5c

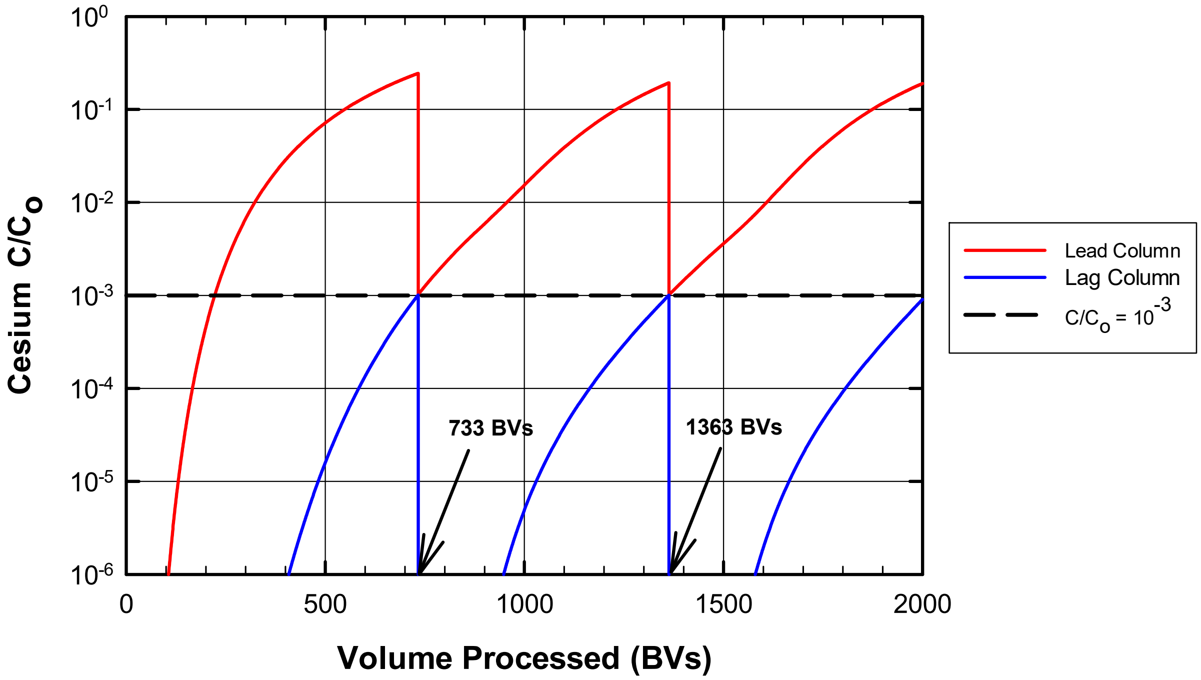

Figure A-48. Case 5c Breakthrough Curves based on Effluent Concentrations

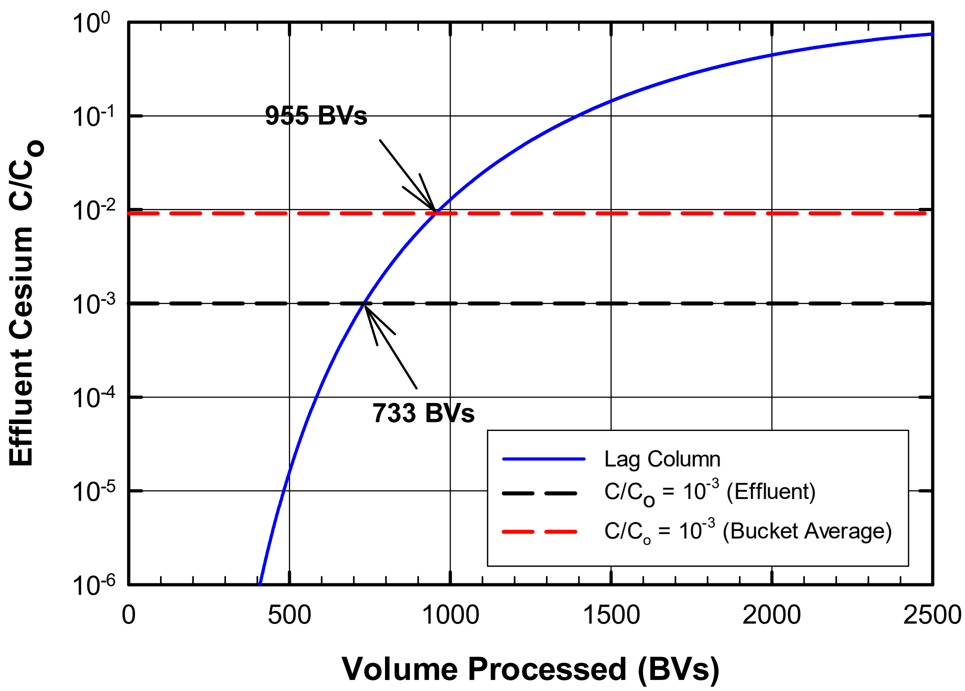

Figure A-49. Case 5c Breakthrough based on Effluent and Bucket-Average Concentrations

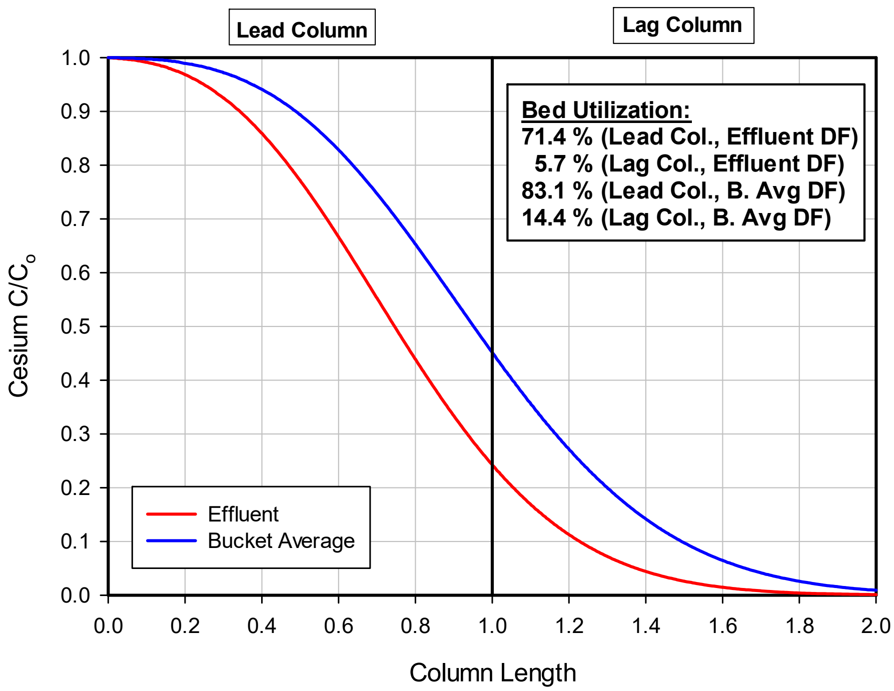

Figure A-50. Case 5c Column Concentration Profiles

Case 5d

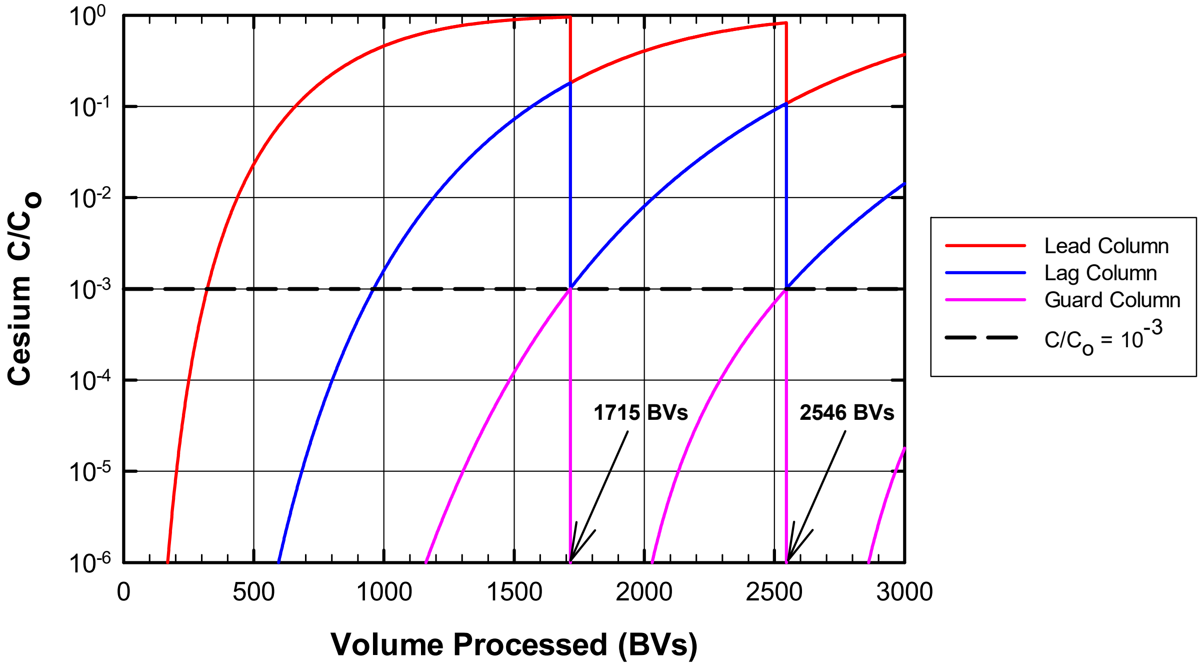

Figure A-51. Case 5d Breakthrough Curves based on Effluent Concentrations

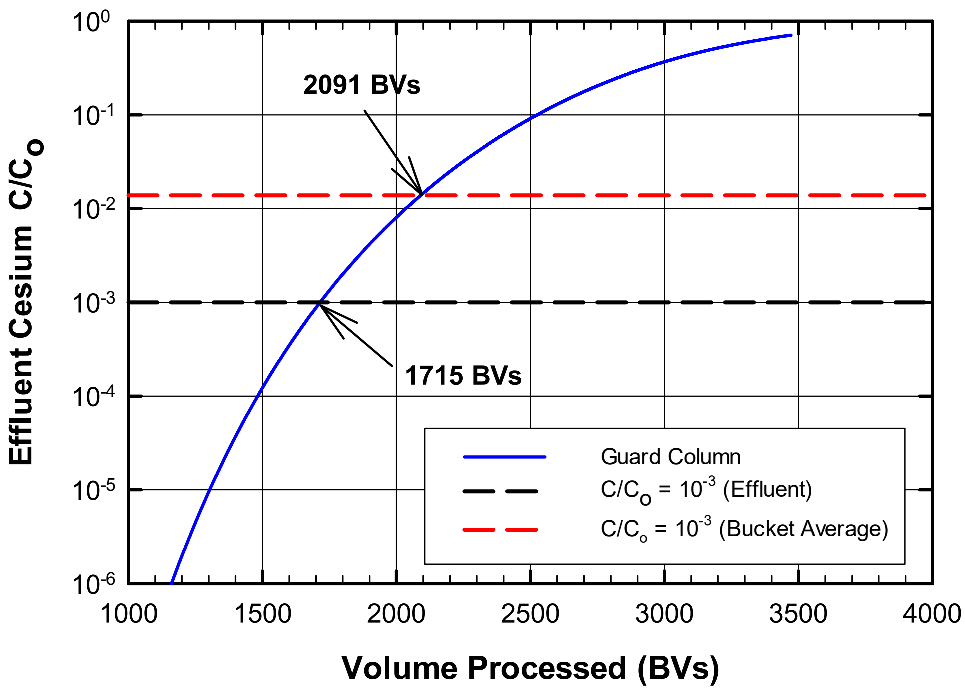

Figure A-52. Case 5d Breakthrough based on Effluent and Bucket-Average Concentrations

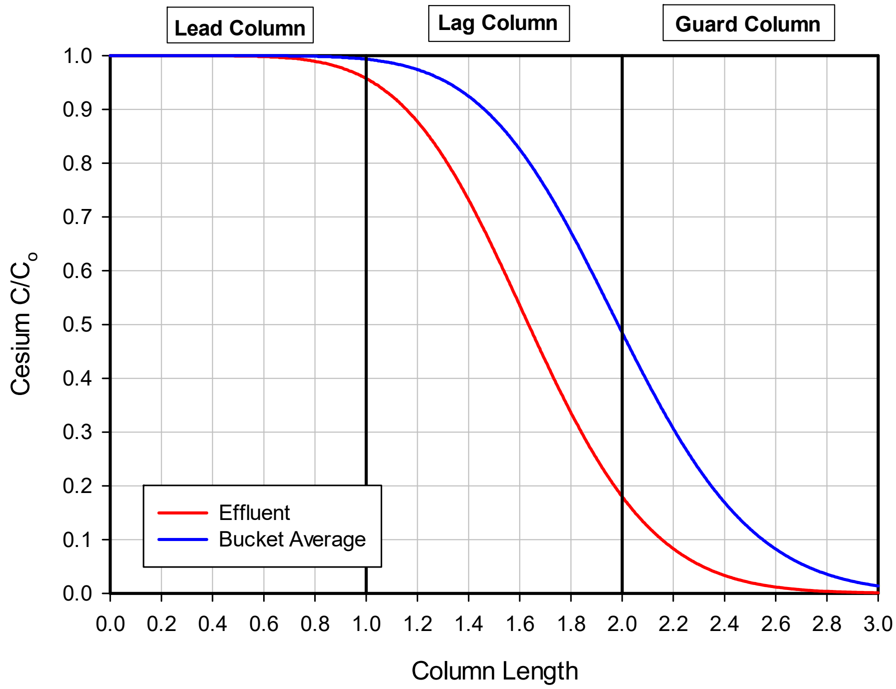

Figure A-53. Case 5d Column Concentration Profiles

Case 5e

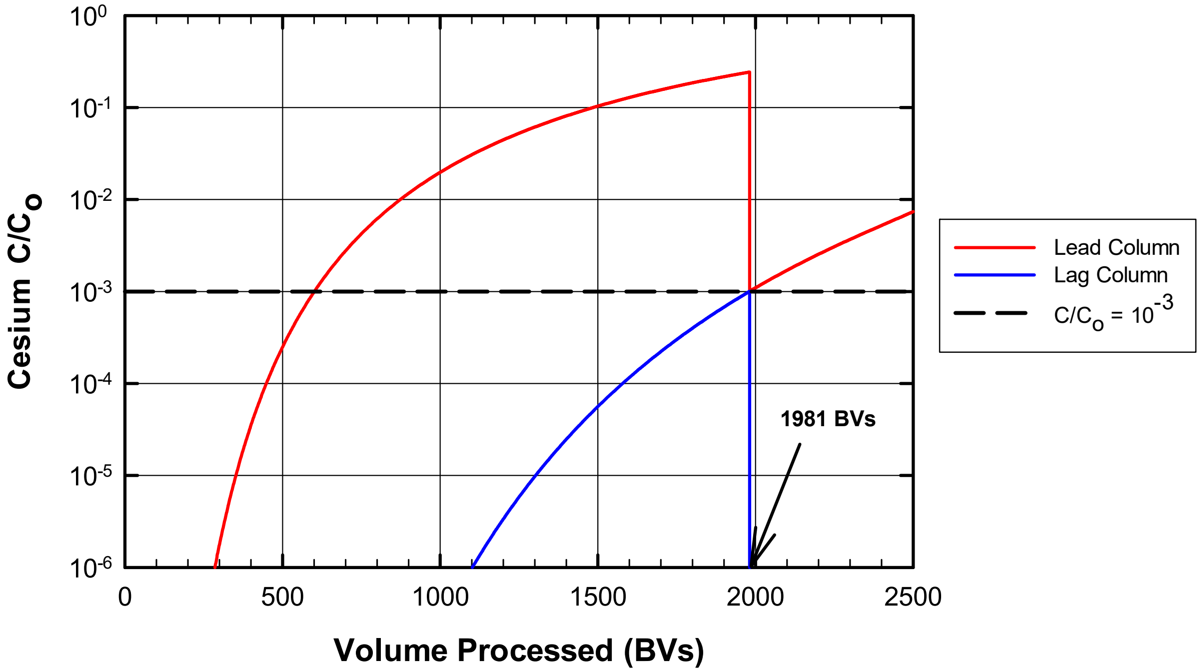

Figure A-54. Case 5e Breakthrough Curves based on Effluent Concentrations

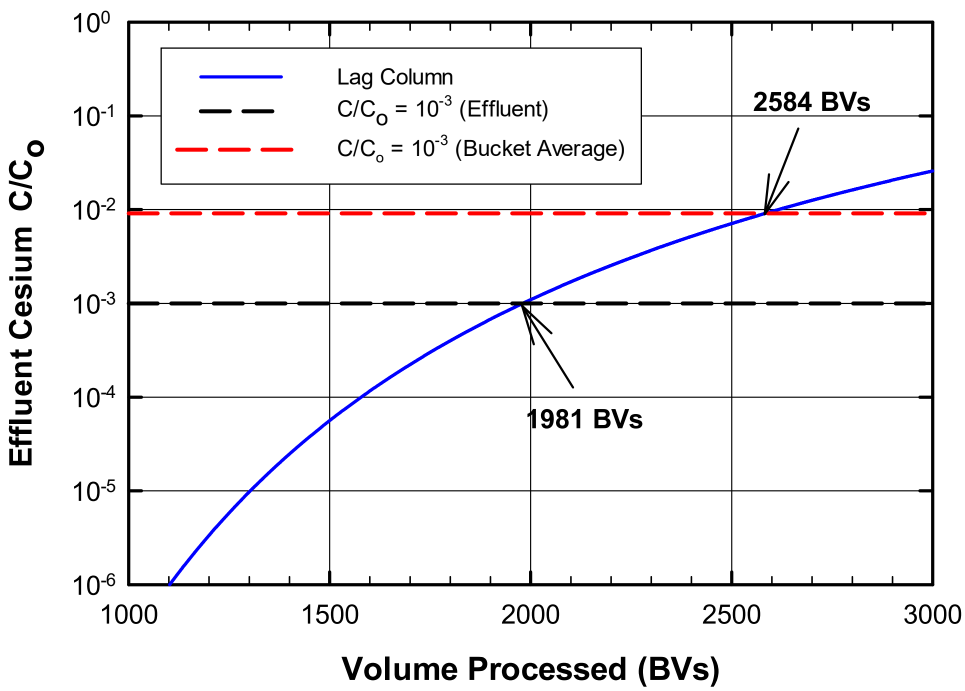

Figure A-55. Case 5e Breakthrough based on Effluent and Bucket-Average Concentrations

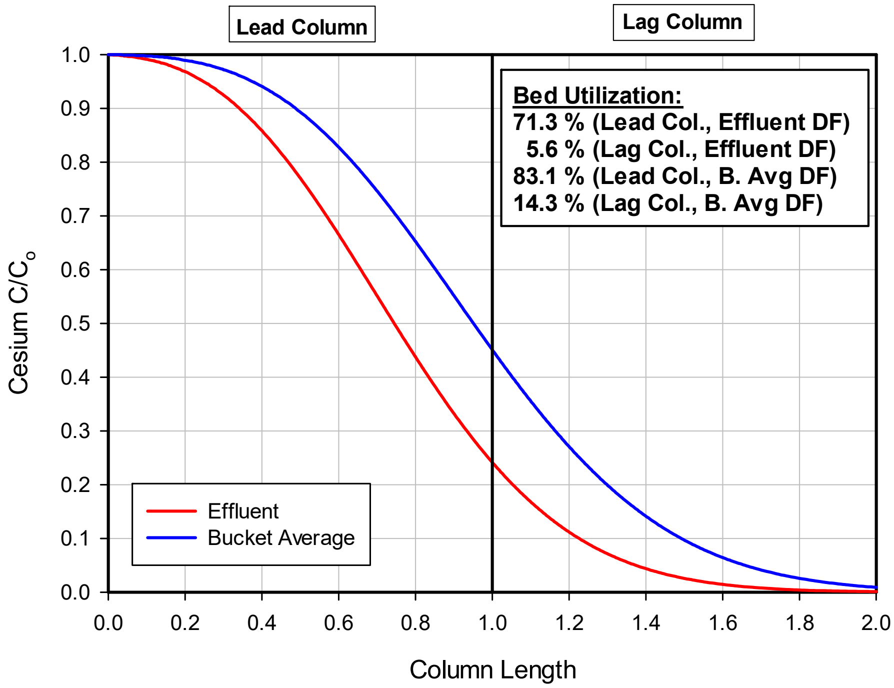

Figure A-56. Case 5e Column Concentration Profiles

Case 5f

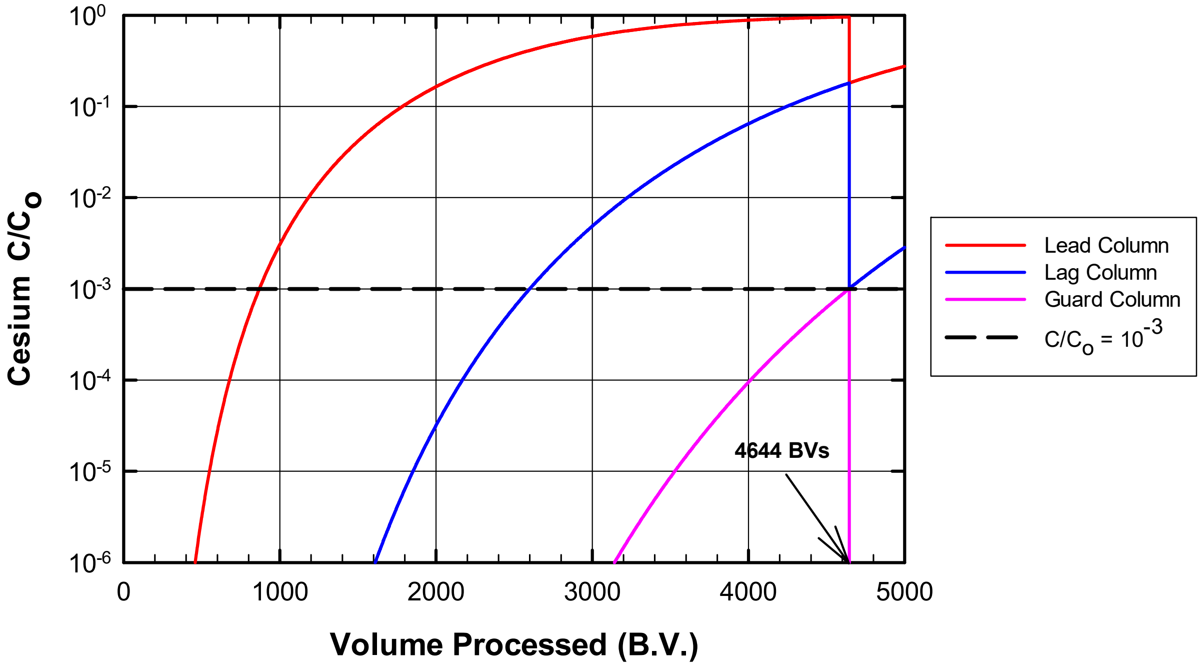

Figure A-57. Case 5f Breakthrough Curves based on Effluent Concentrations

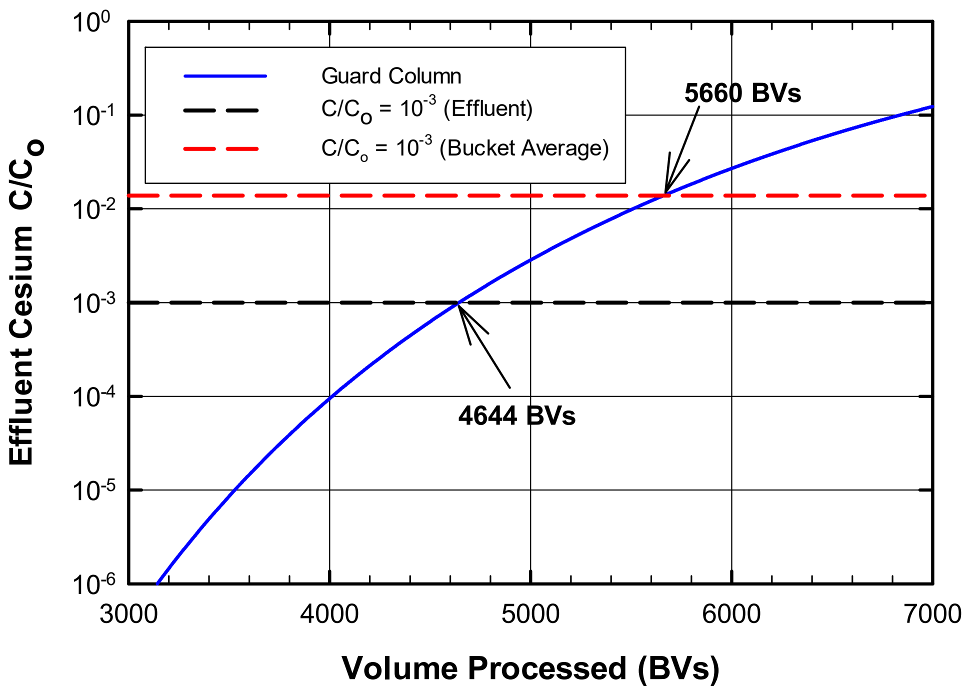

Figure A-58. Case 5f Breakthrough based on Effluent and Bucket-Average Concentrations

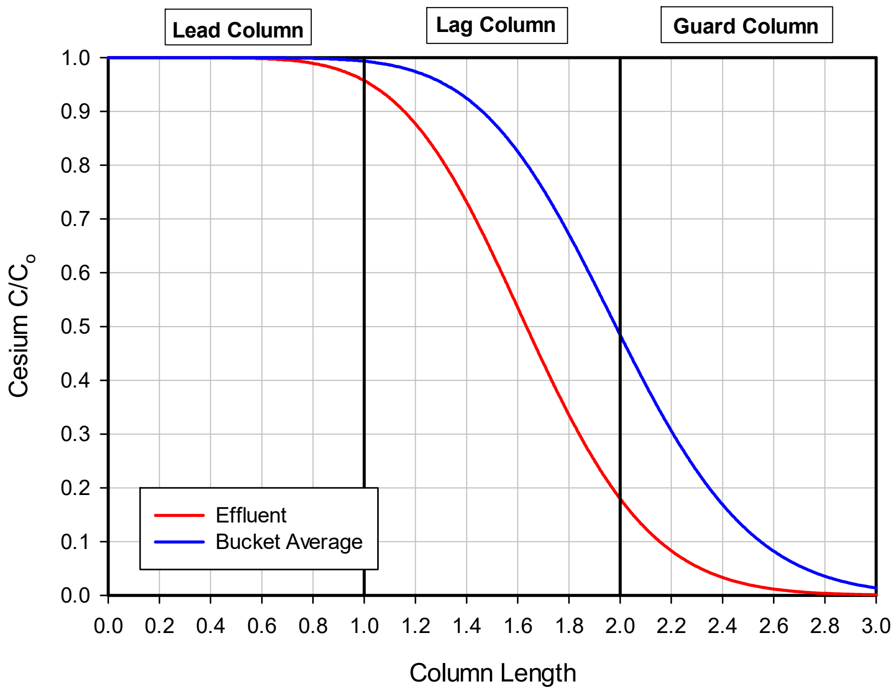

Figure A-59. Case 5f Column Concentration Profiles

Appendix B. VERSE-LC Input and Output Files

Case 1a

VERSE Input:

```
TCCR Simulation of Cs removal on CST material single column
Case 1a - SRS avg simulant, 5 gpm, 35 C, small particle size
1, 50, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
263.59, 48.68, 18927, 6d+4       Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
172.0, 0.50, 0.24,  0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 1.4d-5, 1, 0.0           spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.022, 1.249                     fluid viscosity(poise), density(g/cm^3)
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile at DF=1000 (Effluent)
-1, 7275, 1, 0                   particle point (-1 for all), te, Ne, tr
D                                COMMAND - dump column profile at DF=1000 (Bucket Average)
-1, 9693, 1, 0                   particle point (-1 for all), te, Ne, tr
-                                end of commands
 70000, 1.0                      end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
9.327d-5                         part-pore diffusivities(cm^2/min) 20% of free value
4.663d-4                         Brownian diffusivities(cm^2/min)
0.3395                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5799 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
3.1236d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
===============================================================================

 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF

 ===============================================================================

 Input file: Case1a
 TCCR Simulation of Cs removal on CST material single column
 Case 1a - SRS avg simulant, 5 gpm, 35 C, small particle size
 Begin Run:  14:28:59 on 10-22-2018   running under Windows 95/8
 Finite elements    - axial: 50  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  2010
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 ===============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =  70000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    263.59000 cm          D              =     48.68000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      = 490591.42233 mL
 F              =  18927.00000 mL/min      Uo (linear)    =     20.33859 cm/min
 R              =    172.00000 microns     L/R            =  15325.00000
 Bed Void frac. =       .50000             Pcl. Porosity  =       .24000
 Spec. Area     =     87.20930 1/cm        Time/BV        =     12.96009 min
 Vol CSTRs      =  60000.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .16943E+01
 Dp  [cm2/min]  =  .93270E-04
```

```
Doo [cm2/min]  =  .46630E-03
kf  [cm/min]   =  .26851E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .33101E+00
Sc(i)          =  .22664E+04
Peb(i)         =  .31642E+04
Bi(i)          =  .20632E+03
Nf(i)          =  .60696E+03
Np(i)          =  .98063E+00
Pep(i)         =  .15628E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .31236E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M

===============================================================================

COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1400E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2200E-01 poise and density to 1.249     g/cm3
  3: Monitor conc. history at stream  2.  Filename = Case1a.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  4: Dump full profile file at  7275.     min
     Execute   1 times, every .0000     mins.
  5: Dump full profile file at  9693.     min
     Execute   1 times, every .0000     mins.

===============================================================================
VERSE-LC finished in  5536 steps.  Average step size 12.64     minutes
End run:  14:31:17 on 10-22-2018
Integrated Areas in History Files:
Case1a.h01                 .602278
```

Case 1b

VERSE Input:

```
TCCR Simulation of Cs removal on CST material single column
Case 1b - SRS avg simulant, 8 gpm, 35 C, small particle size
1, 50, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
263.59, 48.68, 30283, 6d+4       Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
172.0, 0.50, 0.24,  0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 1.4d-5, 1, 0.0           spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.022, 1.249                     fluid viscosity(poise), density(g/cm^3)
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile at DF=1000 (Effluent)
-1, 3216, 1, 0                   particle point (-1 for all), te, Ne, tr
D                                COMMAND - dump column profile at DF=1000 (Bucket Average)
-1, 4402, 1, 0                   particle point (-1 for all), te, Ne, tr
-                                end of commands
 70000, 1.0                      end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
9.327d-5                         part-pore diffusivities(cm^2/min) 20% of free value
4.663d-4                         Brownian diffusivities(cm^2/min)
0.3395                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5799 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
3.1236d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: Case1b
 TCCR Simulation of Cs removal on CST material single column
 Case 1b - SRS avg simulant, 8 gpm, 35 C, small particle size
 Begin Run:  15:09:36 on 10-22-2018   running under Windows 95/8
 Finite elements    - axial: 50  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  2010
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 ===============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =  70000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    263.59000 cm          D              =     48.68000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      = 490591.42233 mL
 F              =  30283.00000 mL/min      Uo (linear)    =     32.54152 cm/min
 R              =    172.00000 microns     L/R            =  15325.00000
 Bed Void frac. =       .50000             Pcl. Porosity  =       .24000
 Spec. Area     =     87.20930 1/cm        Time/BV        =      8.10011 min
 Vol CSTRs      =  60000.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .26895E+01
 Dp  [cm2/min]  =  .93270E-04
 Doo [cm2/min]  =  .46630E-03
 kf  [cm/min]   =  .31405E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .52961E+00
 Sc(i)          =  .22664E+04
 Peb(i)         =  .31892E+04
 Bi(i)          =  .24131E+03
```

```
Nf(i)          =  .44369E+03
Np(i)          =  .61290E+00
Pep(i)         =  .25004E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .31236E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1400E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2200E-01 poise and density to 1.249     g/cm3
  3: Monitor conc. history at stream  2.  Filename = Case1b.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  4: Dump full profile file at  3216.     min
     Execute   1 times, every .0000     mins.
  5: Dump full profile file at  4402.     min
     Execute   1 times, every .0000     mins.
===============================================================================
VERSE-LC finished in  8779 steps.  Average step size 7.974     minutes
End run:  15:13:02 on 10-22-2018
Integrated Areas in History Files:
Case1b.h01                 .743898
```

Case 1c

VERSE Input:

```
TCCR Simulation of Cs removal on CST material single column
Case 1c - SRS avg simulant, 10 gpm, 35 C, small particle size
1, 50, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
263.59, 48.68, 37854, 6d+4       Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
172.0, 0.50, 0.24,  0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 1.4d-5, 1, 0.0           spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.022, 1.249                     fluid viscosity(poise), density(g/cm^3)
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile at DF=1000 (Effluent)
-1, 2150, 1, 0                   particle point (-1 for all), te, Ne, tr
D                                COMMAND - dump column profile at DF=1000 (Bucket Average)
-1, 2968, 1, 0                   particle point (-1 for all), te, Ne, tr
-                                end of commands
 70000, 1.0                      end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
9.327d-5                         part-pore diffusivities(cm^2/min) 20% of free value
4.663d-4                         Brownian diffusivities(cm^2/min)
0.3395                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5799 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
3.1236d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: Case1c
 TCCR Simulation of Cs removal on CST material single column
 Case 1c - SRS avg simulant, 10 gpm, 35 C, small particle size
 Begin Run:  15:45:49 on 10-22-2018   running under Windows 95/8
 Finite elements    - axial: 50  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  2010
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 ===============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =  70000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    263.59000 cm          D              =     48.68000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      = 490591.42233 mL
 F              =  37854.00000 mL/min      Uo (linear)    =     40.67717 cm/min
 R              =    172.00000 microns     L/R            =  15325.00000
 Bed Void frac. =       .50000             Pcl. Porosity  =       .24000
 Spec. Area     =     87.20930 1/cm        Time/BV        =      6.48005 min
 Vol CSTRs      =  60000.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .33472E+01
 Dp  [cm2/min]  =  .93270E-04
 Doo [cm2/min]  =  .46630E-03
 kf  [cm/min]   =  .33830E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .66201E+00
 Sc(i)          =  .22664E+04
 Peb(i)         =  .32033E+04
 Bi(i)          =  .25994E+03
```

```
Nf(i)          =  .38236E+03
Np(i)          =  .49031E+00
Pep(i)         =  .31255E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .31236E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1400E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2200E-01 poise and density to 1.249     g/cm3
  3: Monitor conc. history at stream  2.  Filename = Case1c.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  4: Dump full profile file at  2150.     min
     Execute   1 times, every .0000     mins.
  5: Dump full profile file at  2968.     min
     Execute   1 times, every .0000     mins.
===============================================================================
VERSE-LC finished in 10945 steps.  Average step size 6.396     minutes
End run:  15:49:58 on 10-22-2018
Integrated Areas in History Files:
Case1c.h01                 .791120
```

Case 1d

VERSE Input:

```
TCCR Simulation of Cs removal on CST material single column
Case 1d - SRS avg simulant, 5 gpm, 25 C, small particle size
1, 50, 4, 6                       ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                 comp-conc units
263.59, 48.68, 18927, 6d+4        Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
172.0, 0.50, 0.24,  0.0           part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentrations (M)
S                                 COMMAND - inlet conc step change
1, 0.0, 1.4d-5, 1, 0.0            spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.0278, 1.250                     fluid viscosity(poise), density(g/cm^3)
h                                 COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5            unit op#, ptscale(1-4) filtering
D                                 COMMAND - dump column profile at DF=1000 (Effluent)
-1,  9039, 1, 0                   particle point (-1 for all), te, Ne, tr
D                                 COMMAND - dump column profile at DF=1000 (Bucket Average)
-1, 12084, 1, 0                   particle point (-1 for all), te, Ne, tr
-                                 end of commands
 70000, 1.0                       end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                    abs-tol, rel-tol
-                                 non-negative conc constraint
1.0d0                             size exclusion factor
8.885d-5                          part-pore diffusivities(cm^2/min) 20% of free value
4.442d-4                          Brownian diffusivities(cm^2/min)
0.3395                            Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                               Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                               Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5799 x rhob
1.0                               Freundlich/Langmuir Hybrid Mb   (-)
2.4236d-4                         Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
 ==============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ==============================================================================
 Input file: Case1d
 TCCR Simulation of Cs removal on CST material single column
 Case 1d - SRS avg simulant, 5 gpm, 25 C, small particle size
 Begin Run:  16:10:53 on 10-22-2018   running under Windows 95/8
 Finite elements    - axial: 50  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  2010
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 ==============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =  70000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    263.59000 cm          D              =     48.68000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      = 490591.42233 mL
 F              =  18927.00000 mL/min      Uo (linear)    =     20.33859 cm/min
 R              =    172.00000 microns     L/R            =  15325.00000
 Bed Void frac. =       .50000             Pcl. Porosity  =       .24000
 Spec. Area     =     87.20930 1/cm        Time/BV        =     12.96009 min
 Vol CSTRs      =  60000.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .16999E+01
 Dp  [cm2/min]  =  .88850E-04
 Doo [cm2/min]  =  .44420E-03
 kf  [cm/min]   =  .25996E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .26216E+00
 Sc(i)          =  .30041E+04
 Peb(i)         =  .31537E+04
 Bi(i)          =  .20968E+03
```

```
Nf(i)          =  .58763E+03
Np(i)          =  .93416E+00
Pep(i)         =  .16405E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .24236E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1400E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2780E-01 poise and density to 1.250     g/cm3
  3: Monitor conc. history at stream  2.  Filename = Case1d.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  4: Dump full profile file at  9039.     min
     Execute   1 times, every .0000     mins.
  5: Dump full profile file at  .1208E+05 min
     Execute   1 times, every .0000     mins.
===============================================================================
VERSE-LC finished in  5540 steps.  Average step size 12.64     minutes
End run:  16:13:05 on 10-22-2018
Integrated Areas in History Files:
Case1d.h01                 .500130
```

Case 1e

VERSE Input:

```
TCCR Simulation of Cs removal on CST material single column
Case 1e - SRS avg simulant, 5 gpm, 35 C, large particle size
1, 50, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
263.59, 48.68, 18927, 6d+4       Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.50, 0.24,  0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 1.4d-5, 1, 0.0           spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.022, 1.249                     fluid viscosity(poise), density(g/cm^3)
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile at DF=1000 (Effluent)
-1, 3201, 1, 0                   particle point (-1 for all), te, Ne, tr
D                                COMMAND - dump column profile at DF=1000 (Bucket Average)
-1, 4484, 1, 0                   particle point (-1 for all), te, Ne, tr
-                                end of commands
 70000, 1.0                      end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
9.327d-5                         part-pore diffusivities(cm^2/min) 20% of free value
4.663d-4                         Brownian diffusivities(cm^2/min)
0.3395                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5799 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
3.1236d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: Case1e
TCCR Simulation of Cs removal on CST material single column
Case 1e - SRS avg simulant, 5 gpm, 35 C, large particle size
Begin Run:  16:32:26 on 10-22-2018   running under Windows 95/8
Finite elements    - axial: 50  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  2010
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? N   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
===============================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        =  70000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    263.59000 cm          D              =     48.68000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      = 490591.42233 mL
F              =  18927.00000 mL/min      Uo (linear)    =     20.33859 cm/min
R              =    286.00000 microns     L/R            =   9216.43357
Bed Void frac. =       .50000             Pcl. Porosity  =       .24000
Spec. Area     =     52.44755 1/cm        Time/BV        =     12.96009 min
Vol CSTRs      =  60000.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .27931E+01
Dp  [cm2/min]  =  .93270E-04
Doo [cm2/min]  =  .46630E-03
kf  [cm/min]   =  .19131E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .55040E+00
Sc(i)          =  .22664E+04
Peb(i)         =  .19194E+04
Bi(i)          =  .24443E+03
```

```
Nf(i)          =  .26007E+03
Np(i)          =  .35467E+00
Pep(i)         =  .25986E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .31236E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1400E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2200E-01 poise and density to 1.249     g/cm3
  3: Monitor conc. history at stream  2.  Filename = Case1e.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  4: Dump full profile file at  3201.     min
     Execute   1 times, every .0000     mins.
  5: Dump full profile file at  4484.     min
     Execute   1 times, every .0000     mins.
===============================================================================
VERSE-LC finished in  5533 steps.  Average step size 12.65     minutes
End run:  16:34:38 on 10-22-2018
Integrated Areas in History Files:
Case1e.h01                 .605621
```

Case 1f

VERSE Input:

```
TCCR Simulation of Cs removal on CST material single column
Case 1f - Tank 10 projected composition, 5 gpm, 35 C, large particle size
1, 50, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
263.59, 48.68, 18927, 6d+4       Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.50, 0.24,  0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 2.16d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.02494, 1.327                   fluid viscosity(poise), density(g/cm^3)
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile at DF=1000 (Effluent)
-1,  962, 1, 0                   particle point (-1 for all), te, Ne, tr
D                                COMMAND - dump column profile at DF=1000 (Bucket Average)
-1, 1363, 1, 0                   particle point (-1 for all), te, Ne, tr
-                                end of commands
 70000, 1.0                      end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
7.012d-5                         part-pore diffusivities(cm^2/min) 20% of free value
3.506d-4                         Brownian diffusivities(cm^2/min)
0.3395                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5798 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
8.1004d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: Case1f
TCCR Simulation of Cs removal on CST material single column
Case 1f - Tank 10 projected composition, 5 gpm, 35 C, large particle size
Begin Run:  12:23:50 on 10-23-2018   running under Windows 95/8
Finite elements    - axial: 50  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  2010
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? N   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
===============================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        =  70000.00000 min        dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
Total Length   =    263.59000 cm         D              =     48.68000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     = 490591.42233 mL
F              =  18927.00000 mL/min     Uo (linear)    =     20.33859 cm/min
R              =    286.00000 microns    L/R            =   9216.43357
Bed Void frac. =       .50000            Pcl. Porosity  =       .24000
Spec. Area     =     52.44755 1/cm       Time/BV        =     12.96009 min
Vol CSTRs      =  60000.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .27965E+01
Dp  [cm2/min]  =  .70120E-04
Doo [cm2/min]  =  .35060E-03
kf  [cm/min]   =  .15818E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .51583E+00
Sc(i)          =  .32164E+04
Peb(i)         =  .19171E+04
```

```
Bi(i)          =  .26883E+03
Nf(i)          =  .21504E+03
Np(i)          =  .26664E+00
Pep(i)         =  .34565E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .81004E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .2160E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2494E-01 poise and density to 1.327     g/cm3
  3: Monitor conc. history at stream  2.  Filename = Case1f.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  4: Dump full profile file at  962.0     min
     Execute   1 times, every .0000     mins.
  5: Dump full profile file at  1363.     min
     Execute   1 times, every .0000     mins.
===============================================================================
VERSE-LC finished in  5521 steps.  Average step size 12.68     minutes
End run:  12:25:58 on 10-23-2018
Integrated Areas in History Files:
Case1f.h01                 1.28303
```

Case 2a

VERSE Input:

```
TCCR Simulation of Cs removal on CST material single column
Case 2a - SRS avg simulant, 3 gpm, 35 C, large particle size
1, 50, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNA                           isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                           input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                               comp-conc units
263.59, 48.68, 11356, 6d+4      Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.50, 0.24,  0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                             initial concentrations (M)
S                               COMMAND - inlet conc step change
1, 0.0, 1.4d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                               COMMAND - viscosity/density change
0.022, 1.249                    fluid viscosity(poise), density(g/cm^3)
h                               COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5          unit op#, ptscale(1-4) filtering
D                               COMMAND - dump column profile at DF=1000 (Effluent)
-1,  8220, 1, 0                 particle point (-1 for all), te, Ne, tr
D                               COMMAND - dump column profile at DF=1000 (Bucket Average)
-1, 11300, 1, 0                 particle point (-1 for all), te, Ne, tr
-                               end of commands
 70000, 1.0                     end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                  abs-tol, rel-tol
-                               non-negative conc constraint
1.0d0                           size exclusion factor
9.327d-5                        part-pore diffusivities(cm^2/min) 20% of free value
4.663d-4                        Brownian diffusivities(cm^2/min)
0.3395                          Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                             Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                             Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5799 x rhob
1.0                             Freundlich/Langmuir Hybrid Mb   (-)
3.1236d-4                       Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
 ==============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ==============================================================================
 Input file: Case2a
 TCCR Simulation of Cs removal on CST material single column
 Case 2a - SRS avg simulant, 3 gpm, 35 C, large particle size
 Begin Run:  16:12:34 on 11-07-2018   running under Windows 95/8
 Finite elements    - axial: 50  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  2010
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 ==============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =  70000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    263.59000 cm          D              =     48.68000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      = 490591.42233 mL
 F              =  11356.00000 mL/min      Uo (linear)    =     12.20294 cm/min
 R              =    286.00000 microns     L/R            =   9216.43357
 Bed Void frac. =       .50000             Pcl. Porosity  =       .24000
 Spec. Area     =     52.44755 1/cm        Time/BV        =     21.60054 min
 Vol CSTRs      =  60000.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .16904E+01
 Dp  [cm2/min]  =  .93270E-04
 Doo [cm2/min]  =  .46630E-03
 kf  [cm/min]   =  .16135E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .33023E+00
 Sc(i)          =  .22664E+04
 Peb(i)         =  .19029E+04
 Bi(i)          =  .20615E+03
```

```
Nf(i)          =  .36560E+03
Np(i)          =  .59113E+00
Pep(i)         =  .15591E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .31236E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
==============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1400E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2200E-01 poise and density to 1.249     g/cm3
  3: Monitor conc. history at stream  2.  Filename = Case2a.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  4: Dump full profile file at  8220.     min
     Execute   1 times, every .0000     mins.
  5: Dump full profile file at  .1130E+05 min
     Execute   1 times, every .0000     mins.
==============================================================================
VERSE-LC finished in  3379 steps.  Average step size 20.72     minutes
End run:  16:14:40 on 11-07-2018
Integrated Areas in History Files:
Case2a.h01                 .376451
```

Case 2b

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead lag guard columns
Case 2b - SRS avg simulant, 3 gpm, 35 C, large particle size
1, 150, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNF                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
790.77, 48.68, 11356, 0d+0       Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.50, 0.24,  0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 1.4d-5, 1, 0.0           spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.022, 1.249                     fluid viscosity(poise), density(g/cm^3)
m                                COMMAND - subcolumns (carousel-concentration driven)
50, 150, 0, 1, 1.4d-8, 0.0, 70000    Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile (Col #1 Breakthrough)
-1,  8202, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #2 Breakthrough)
-1, 27433, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #3 Breakthrough)
-1, 52303, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
-                                end of commands
70000, 1                         end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
9.327d-5                         part-pore diffusivities(cm^2/min) 20% of free value
4.663d-4                         Brownian diffusivities(cm^2/min)
0.3395                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5799 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
3.1236d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
 ==============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ==============================================================================
 Input file: Case2b
 TCCR Simulation of Cs removal on CST material lead lag guard columns
 Case 2b - SRS avg simulant, 3 gpm, 35 C, large particle size
 Begin Run:  11:04:23 on 11-10-2018   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6010
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 Sub-Column Boundary Conditions: Flux Continuity
 ==============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =  70000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    790.77000 cm          D              =     48.68000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =1471774.26698 mL
 F              =  11356.00000 mL/min      Uo (linear)    =     12.20294 cm/min
 R              =    286.00000 microns     L/R            =  27649.30070
 Bed Void frac. =       .50000             Pcl. Porosity  =       .24000
 Spec. Area     =     52.44755 1/cm        Time/BV        =     21.60054 min
 Vol CSTRs      =       .00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .16904E+01
 Dp  [cm2/min]  =  .93270E-04
```

```
Doo [cm2/min]  =  .46630E-03
kf  [cm/min]   =  .16135E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .33023E+00
Sc(i)          =  .22664E+04
Peb(i)         =  .19029E+04
Bi(i)          =  .20615E+03
Nf(i)          =  .36560E+03
Np(i)          =  .59113E+00
Pep(i)         =  .15591E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .31236E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1400E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2200E-01 poise and density to 1.249     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .7000E+05 min.
     When comp.  1 reaches .1400E-07 M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case2b.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case2b.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = Case2b.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  7: Dump full profile file at  8202.     min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  .2743E+05 min
     Execute   1 times, every .0000     mins.
  9: Dump full profile file at  .5230E+05 min
     Execute   1 times, every .0000     mins.
===============================================================================
Conc. Carousel caused bed shift at t = .5232E+05 min
VERSE-LC finished in  3264 steps.  Average step size 21.45     minutes
End run:  11:05:14 on 11-10-2018
Integrated Areas in History Files:
Case2b.h01                .220970
Case2b.h02                .995183E-02
Case2b.h03                .641023E-04
```

Case 2c

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead lag guard columns
Case 2c - SRS avg simulant, 5 gpm, 35 C, large particle size
1, 150, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNF                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
790.77, 48.68, 18927, 0.0d+0     Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.50, 0.24,  0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 1.4d-5, 1, 0.0           spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.022, 1.249                     fluid viscosity(poise), density(g/cm^3)
m                                COMMAND - subcolumns (carousel-concentration driven)
50, 150, 0, 1, 1.4d-8, 0.0, 70000    Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile (Col #1 Breakthrough)
-1,  3189, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #2 Breakthrough)
-1, 11546, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #3 Breakthrough)
-1, 23215, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
-                                end of commands
70000, 1                         end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
9.327d-5                         part-pore diffusivities(cm^2/min) 20% of free value
4.663d-4                         Brownian diffusivities(cm^2/min)
0.3395                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5799 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
3.1236d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: Case2c
 TCCR Simulation of Cs removal on CST material lead lag guard columns
 Case 2c - SRS avg simulant, 5 gpm, 35 C, large particle size
 Begin Run:  21:51:54 on 11-11-2018   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6010
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 Sub-Column Boundary Conditions: Flux Continuity
 ===============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =  70000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    790.77000 cm          D              =     48.68000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =1471774.26698 mL
 F              =  18927.00000 mL/min      Uo (linear)    =     20.33859 cm/min
 R              =    286.00000 microns     L/R            =  27649.30070
 Bed Void frac. =       .50000             Pcl. Porosity  =       .24000
 Spec. Area     =     52.44755 1/cm        Time/BV        =     12.96009 min
 Vol CSTRs      =       .00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .27931E+01
 Dp  [cm2/min]  =  .93270E-04
```

```
Doo [cm2/min]  =  .46630E-03
kf  [cm/min]   =  .19131E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .55040E+00
Sc(i)          =  .22664E+04
Peb(i)         =  .19194E+04
Bi(i)          =  .24443E+03
Nf(i)          =  .26007E+03
Np(i)          =  .35467E+00
Pep(i)         =  .25986E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .31236E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1400E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2200E-01 poise and density to 1.249     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .7000E+05 min.
     When comp.  1 reaches .1400E-07 M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case2c.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case2c.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = Case2c.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  7: Dump full profile file at  3189.     min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  .1155E+05 min
     Execute   1 times, every .0000     mins.
  9: Dump full profile file at  .2322E+05 min
     Execute   1 times, every .0000     mins.
===============================================================================
Conc. Carousel caused bed shift at t = .2323E+05 min
Conc. Carousel caused bed shift at t = .3736E+05 min
Conc. Carousel caused bed shift at t = .5287E+05 min
Conc. Carousel caused bed shift at t = .6883E+05 min
VERSE-LC finished in  5438 steps.  Average step size 12.87     minutes
End run:  21:53:18 on 11-11-2018
Integrated Areas in History Files:
Case2c.h01                 .159928
Case2c.h02                 .847825E-02
Case2c.h03                 .169199E-03
```

Case 2d

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead lag guard columns
Case 2d - SRS avg simulant, 8 gpm, 35 C, large particle size
1, 150, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNF                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
790.77, 48.68, 30283, 0.0d+0     Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.50, 0.24,  0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 1.4d-5, 1, 0.0           spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.022, 1.249                     fluid viscosity(poise), density(g/cm^3)
m                                COMMAND - subcolumns (carousel-concentration driven)
50, 150, 0, 1, 1.4d-8, 0.0, 70000    Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile (Col #1 Breakthrough)
-1,  1277, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #2 Breakthrough)
-1,  4950, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #3 Breakthrough)
-1, 10386, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
-                                end of commands
70000, 1                         end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
9.327d-5                         part-pore diffusivities(cm^2/min) 20% of free value
4.663d-4                         Brownian diffusivities(cm^2/min)
0.3395                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5799 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
3.1236d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: Case2d
TCCR Simulation of Cs removal on CST material lead lag guard columns
Case 2d - SRS avg simulant, 8 gpm, 35 C, large particle size
Begin Run:  21:48:04 on 11-11-2018   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6010
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? N   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
Sub-Column Boundary Conditions: Flux Continuity
===============================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        =  70000.00000 min        dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
Total Length   =    790.77000 cm         D              =     48.68000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =1471774.26698 mL
F              =  30283.00000 mL/min     Uo (linear)    =     32.54152 cm/min
R              =    286.00000 microns    L/R            =  27649.30070
Bed Void frac. =       .50000            Pcl. Porosity  =       .24000
Spec. Area     =     52.44755 1/cm       Time/BV        =      8.10011 min
Vol CSTRs      =       .00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .44245E+01
Dp  [cm2/min]  =  .93270E-04
```

```
Doo [cm2/min]  =  .46630E-03
kf  [cm/min]   =  .22375E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .88063E+00
Sc(i)          =  .22664E+04
Peb(i)         =  .19387E+04
Bi(i)          =  .28588E+03
Nf(i)          =  .19012E+03
Np(i)          =  .22167E+00
Pep(i)         =  .41577E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .31236E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1400E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2200E-01 poise and density to 1.249     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .7000E+05 min.
     When comp.  1 reaches .1400E-07 M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case2d.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case2d.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = Case2d.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  7: Dump full profile file at  1277.     min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  4950.     min
     Execute   1 times, every .0000     mins.
  9: Dump full profile file at  .1039E+05 min
     Execute   1 times, every .0000     mins.
===============================================================================
Conc. Carousel caused bed shift at t = .1039E+05 min
Conc. Carousel caused bed shift at t = .1726E+05 min
Conc. Carousel caused bed shift at t = .2477E+05 min
Conc. Carousel caused bed shift at t = .3235E+05 min
Conc. Carousel caused bed shift at t = .3990E+05 min
Conc. Carousel caused bed shift at t = .4746E+05 min
Conc. Carousel caused bed shift at t = .5501E+05 min
Conc. Carousel caused bed shift at t = .6256E+05 min
VERSE-LC finished in  8715 steps.  Average step size 8.032     minutes
End run:  21:50:21 on 11-11-2018
Integrated Areas in History Files:
Case2d.h01                 .137084
Case2d.h02                 .753380E-02
Case2d.h03                 .208174E-03
```

Case 2e

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead lag guard columns
Case 2e - SRS avg simulant, 2 gpm, 35 C, large particle size
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNF                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                 comp-conc units
790.77, 48.68, 7571, 0.0d+0       Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.50, 0.24,  0.0           part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentrations (M)
S                                 COMMAND - inlet conc step change
1, 0.0, 1.4d-5, 1, 0.0            spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.022, 1.249                      fluid viscosity(poise), density(g/cm^3)
m                                 COMMAND - subcolumns (carousel-concentration driven)
50, 150, 0, 1, 1.4d-8, 0.0, 150000   Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                 COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5            unit op#, ptscale(1-4) filtering
D                                 COMMAND - dump column profile (Col #1 Breakthrough)
-1, 16713, 1, 0                   particle point (-1 for all), time(min), freq, dt(min)
D                                 COMMAND - dump column profile (Col #2 Breakthrough)
-1, 52020, 1, 0                   particle point (-1 for all), time(min), freq, dt(min)
D                                 COMMAND - dump column profile (Col #3 Breakthrough)
-1, 95038, 1, 0                   particle point (-1 for all), time(min), freq, dt(min)
-                                 end of commands
150000, 1                         end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                    abs-tol, rel-tol
-                                 non-negative conc constraint
1.0d0                             size exclusion factor
9.327d-5                          part-pore diffusivities(cm^2/min) 20% of free value
4.663d-4                          Brownian diffusivities(cm^2/min)
0.3395                            Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                               Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                               Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5799 x rhob
1.0                               Freundlich/Langmuir Hybrid Mb   (-)
3.1236d-4                         Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
==============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
==============================================================================
Input file: Case2e
TCCR Simulation of Cs removal on CST material lead lag guard columns
Case 2e - SRS avg simulant, 2 gpm, 35 C, large particle size
Begin Run:  21:43:04 on 11-11-2018   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6010
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? N   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
Sub-Column Boundary Conditions: Flux Continuity
==============================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        = 150000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    790.77000 cm          D              =     48.68000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =1471774.26698 mL
F              =   7571.00000 mL/min      Uo (linear)    =      8.13565 cm/min
R              =    286.00000 microns     L/R            =  27649.30070
Bed Void frac. =       .50000             Pcl. Porosity  =       .24000
Spec. Area     =     52.44755 1/cm        Time/BV        =     32.39938 min
Vol CSTRs      =       .00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .11333E+01
Dp  [cm2/min]  =  .93270E-04
```

```
Doo [cm2/min]  =  .46630E-03
kf  [cm/min]   =  .14096E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .22016E+00
Sc(i)          =  .22664E+04
Peb(i)         =  .18923E+04
Bi(i)          =  .18010E+03
Nf(i)          =  .47905E+03
Np(i)          =  .88666E+00
Pep(i)         =  .10395E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .31236E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1400E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2200E-01 poise and density to 1.249     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1500E+06 min.
     When comp.  1 reaches .1400E-07 M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case2e.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case2e.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = Case2e.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  7: Dump full profile file at  .1671E+05 min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  .5202E+05 min
     Execute   1 times, every .0000     mins.
  9: Dump full profile file at  .9504E+05 min
     Execute   1 times, every .0000     mins.
===============================================================================
Conc. Carousel caused bed shift at t = .9507E+05 min
Conc. Carousel caused bed shift at t = .1432E+06 min
VERSE-LC finished in  4653 steps.  Average step size 32.24     minutes
End run:  21:44:15 on 11-11-2018
Integrated Areas in History Files:
Case2e.h01                 .677045
Case2e.h02                 .356039E-01
Case2e.h03                 .194761E-03
```

Case 2ee

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead lag guard columns
Case 2ee - SRS avg simulant, 2 gpm, 35 C, large particle size
1, 150, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNF                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
790.77, 48.68, 7571, 0.0d+0      Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.548, 0.24,  0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 1.4d-5, 1, 0.0           spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.022, 1.249                     fluid viscosity(poise), density(g/cm^3)
m                                COMMAND - subcolumns (carousel-concentration driven)
50, 150, 0, 1, 1.4d-8, 0.0, 150000   Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile (Col #1 Breakthrough)
-1, 19479, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #2 Breakthrough)
-1, 59677, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #3 Breakthrough)
-1, 107940, 1, 0                 particle point (-1 for all), time(min), freq, dt(min)
-                                end of commands
150000, 1                        end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
1.166d-4                         part-pore diffusivities(cm^2/min) 25% of free value
4.663d-4                         Brownian diffusivities(cm^2/min)
0.3687                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.935 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5799 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
3.1236d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
 ==============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ==============================================================================
 Input file: Case2ee
 TCCR Simulation of Cs removal on CST material lead lag guard columns
 Case 2ee - SRS avg simulant, 2 gpm, 35 C, large particle size
 Begin Run:  17:13:51 on 11-13-2018   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6010
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 Sub-Column Boundary Conditions: Flux Continuity
 ==============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        = 150000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    790.77000 cm          D              =     48.68000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =1471774.26698 mL
 F              =   7571.00000 mL/min      Uo (linear)    =      7.42304 cm/min
 R              =    286.00000 microns     L/R            =  27649.30070
 Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
 Spec. Area     =     47.41259 1/cm        Time/BV        =     35.50972 min
 Vol CSTRs      =       .00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .11333E+01
 Dp  [cm2/min]  =  .11660E-03
```

```
Doo [cm2/min]  =  .46630E-03
kf  [cm/min]   =  .12861E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .22016E+00
Sc(i)          =  .22664E+04
Peb(i)         =  .17266E+04
Bi(i)          =  .13144E+03
Nf(i)          =  .39513E+03
Np(i)          =  .12149E+01
Pep(i)         =  .75864E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .36870E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .31236E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1400E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2200E-01 poise and density to 1.249     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1500E+06 min.
     When comp.  1 reaches .1400E-07 M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case2ee.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case2ee.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = Case2ee.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  7: Dump full profile file at  .1948E+05 min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  .5968E+05 min
     Execute   1 times, every .0000     mins.
  9: Dump full profile file at  .1079E+06 min
     Execute   1 times, every .0000     mins.
===============================================================================
Conc. Carousel caused bed shift at t = .1080E+06 min
VERSE-LC finished in  4244 steps.  Average step size 35.34     minutes
End run:  17:18:33 on 11-13-2018
Integrated Areas in History Files:
Case2ee.h01                .714338
Case2ee.h02                .347145E-01
Case2ee.h03                .119476E-03
```

Case 2f

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead lag guard columns
Case 2f - Tank 10 projected composition, 2 gpm, 35 C, large particle size
1, 150, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNF                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
790.77, 48.68, 7571, 0.0d+0      Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.50, 0.24,  0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 2.16d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.02494, 1.327                   fluid viscosity(poise), density(g/cm^3)
m                                COMMAND - subcolumns (carousel-concentration driven)
50, 150, 0, 1, 2.16d-8, 0.0, 150000  Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile (Col #1 Breakthrough)
-1,  5244, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #2 Breakthrough)
-1, 17163, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #3 Breakthrough)
-1, 32293, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
-                                end of commands
150000, 1                        end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
7.012d-5                         part-pore diffusivities(cm^2/min) 20% of free value
3.506d-4                         Brownian diffusivities(cm^2/min)
0.3395                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5798 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
8.1004d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: Case2f
TCCR Simulation of Cs removal on CST material lead lag guard columns
Case 2f - Tank 10 projected composition, 2 gpm, 35 C, large particle size
Begin Run:  14:19:39 on 11-13-2018   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6010
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? N   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
Sub-Column Boundary Conditions: Flux Continuity
===============================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        = 150000.00000 min        dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
Total Length   =    790.77000 cm         D              =     48.68000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =1471774.26698 mL
F              =   7571.00000 mL/min     Uo (linear)    =      8.13565 cm/min
R              =    286.00000 microns    L/R            =  27649.30070
Bed Void frac. =       .50000            Pcl. Porosity  =       .24000
Spec. Area     =     52.44755 1/cm       Time/BV        =     32.39938 min
Vol CSTRs      =       .00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .11342E+01
Dp  [cm2/min]  =  .70120E-04
```

```
Doo [cm2/min]  =  .35060E-03
kf  [cm/min]   =  .11655E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .20634E+00
Sc(i)          =  .32164E+04
Peb(i)         =  .18908E+04
Bi(i)          =  .19808E+03
Nf(i)          =  .39611E+03
Np(i)          =  .66659E+00
Pep(i)         =  .13826E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .81004E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .2160E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2494E-01 poise and density to 1.327     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1500E+06 min.
     When comp.  1 reaches .2160E-07 M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case2f.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case2f.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = Case2f.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  7: Dump full profile file at  5244.     min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  .1716E+05 min
     Execute   1 times, every .0000     mins.
  9: Dump full profile file at  .3229E+05 min
     Execute   1 times, every .0000     mins.
===============================================================================
Conc. Carousel caused bed shift at t = .3233E+05 min
Conc. Carousel caused bed shift at t = .4961E+05 min
Conc. Carousel caused bed shift at t = .6807E+05 min
Conc. Carousel caused bed shift at t = .8734E+05 min
Conc. Carousel caused bed shift at t = .1071E+06 min
Conc. Carousel caused bed shift at t = .1270E+06 min
Conc. Carousel caused bed shift at t = .1470E+06 min
VERSE-LC finished in  4683 steps.  Average step size 32.03     minutes
End run:  14:25:04 on 11-13-2018
Integrated Areas in History Files:
Case2f.h01                 .654548
Case2f.h02                 .345510E-01
Case2f.h03                 .520621E-03
```

Case 2ff

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead lag guard columns
Case 2f - Tank 10 projected composition, 2 gpm, 35 C, large particle size
1, 150, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNF                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
790.77, 48.68, 7571, 0.0d+0      Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.548, 0.24,  0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 2.16d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.02494, 1.327                   fluid viscosity(poise), density(g/cm^3)
m                                COMMAND - subcolumns (carousel-concentration driven)
50, 150, 0, 1, 2.16d-8, 0.0, 150000  Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile (Col #1 Breakthrough)
-1,  6142, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #2 Breakthrough)
-1, 19834, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #3 Breakthrough)
-1, 36938, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
-                                end of commands
150000, 1                        end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
8.764d-5                         part-pore diffusivities(cm^2/min) 25% of free value
3.506d-4                         Brownian diffusivities(cm^2/min)
0.3686                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.935 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5798 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
8.1004d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
==============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
==============================================================================
Input file: Case2ff
TCCR Simulation of Cs removal on CST material lead lag guard columns
Case 2f - Tank 10 projected composition, 2 gpm, 35 C, large particle size
Begin Run:  15:15:56 on 11-13-2018   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6010
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? N   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
Sub-Column Boundary Conditions: Flux Continuity
==============================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        = 150000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    790.77000 cm          D              =     48.68000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =1471774.26698 mL
F              =   7571.00000 mL/min      Uo (linear)    =      7.42304 cm/min
R              =    286.00000 microns     L/R            =  27649.30070
Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
Spec. Area     =     47.41259 1/cm        Time/BV        =     35.50972 min
Vol CSTRs      =       .00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .11342E+01
Dp  [cm2/min]  =  .87640E-04
```

```
Doo [cm2/min]  =  .35060E-03
kf  [cm/min]   =  .10634E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .20634E+00
Sc(i)          =  .32164E+04
Peb(i)         =  .17252E+04
Bi(i)          =  .14460E+03
Nf(i)          =  .32672E+03
Np(i)          =  .91312E+00
Pep(i)         =  .10093E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .36860E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .81004E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .2160E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2494E-01 poise and density to 1.327     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1500E+06 min.
     When comp.  1 reaches .2160E-07 M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case2ff.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case2ff.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = Case2ff.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  7: Dump full profile file at  6142.     min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  .1983E+05 min
     Execute   1 times, every .0000     mins.
  9: Dump full profile file at  .3694E+05 min
     Execute   1 times, every .0000     mins.
===============================================================================
Conc. Carousel caused bed shift at t = .3697E+05 min
Conc. Carousel caused bed shift at t = .5632E+05 min
Conc. Carousel caused bed shift at t = .7692E+05 min
Conc. Carousel caused bed shift at t = .9837E+05 min
Conc. Carousel caused bed shift at t = .1204E+06 min
Conc. Carousel caused bed shift at t = .1427E+06 min
VERSE-LC finished in  4271 steps.  Average step size 35.12     minutes
End run:  15:20:54 on 11-13-2018
Integrated Areas in History Files:
Case2ff.h01               .700625
Case2ff.h02               .373493E-01
Case2ff.h03               .472594E-03
```

Case 2g

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead lag guard columns
Case 2g - Tank 10 adjusted VDS sample, 2 gpm, 35 C, large particle size
1, 150, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNF                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
790.77, 48.68, 7571, 0.0d+0      Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.50, 0.24,  0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 2.944d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.02675, 1.2786                  fluid viscosity(poise), density(g/cm^3)
m                                COMMAND - subcolumns (carousel-concentration driven)
50, 150, 0, 1, 2.944d-8, 0.0, 1E6    Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile (Col #1 Breakthrough)
-1, 14947, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #2 Breakthrough)
-1, 49938, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #3 Breakthrough)
-1, 95134, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
-                                end of commands
160000, 1                        end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
6.244d-5                         part-pore diffusivities(cm^2/min) 20% of free value
3.122d-4                         Brownian diffusivities(cm^2/min)
0.3395                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5799 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
2.5583d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
 ==============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ==============================================================================
 Input file: Case2g
 TCCR Simulation of Cs removal on CST material lead lag guard columns
 Case 2g - Tank 10 adjusted VDS sample, 2 gpm, 35 C, large particle size
 Begin Run:  16:31:26 on 11-14-2018   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6010
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 Sub-Column Boundary Conditions: Flux Continuity
 ==============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        = 160000.00000 min        dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
 Total Length   =    790.77000 cm         D              =     48.68000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =1471774.26698 mL
 F              =   7571.00000 mL/min     Uo (linear)    =      8.13565 cm/min
 R              =    286.00000 microns    L/R            =  27649.30070
 Bed Void frac. =       .50000            Pcl. Porosity  =       .24000
 Spec. Area     =     52.44755 1/cm       Time/BV        =     32.39938 min
 Vol CSTRs      =       .00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .11356E+01
 Dp  [cm2/min]  =  .62440E-04
```

```
Doo [cm2/min]  =  .31220E-03
kf  [cm/min]   =  .10788E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .18536E+00
Sc(i)          =  .40208E+04
Peb(i)         =  .18884E+04
Bi(i)          =  .20589E+03
Nf(i)          =  .36663E+03
Np(i)          =  .59358E+00
Pep(i)         =  .15527E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .25583E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .2944E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2675E-01 poise and density to 1.279     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .2944E-07 M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case2g.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case2g.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = Case2g.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  7: Dump full profile file at  .1495E+05 min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  .4994E+05 min
     Execute   1 times, every .0000     mins.
  9: Dump full profile file at  .9513E+05 min
     Execute   1 times, every .0000     mins.
===============================================================================
Conc. Carousel caused bed shift at t = .9517E+05 min
Conc. Carousel caused bed shift at t = .1472E+06 min
VERSE-LC finished in  4972 steps.  Average step size 32.18     minutes
End run:  16:36:59 on 11-14-2018
Integrated Areas in History Files:
Case2g.h01                1.18825
Case2g.h02                .587200E-01
Case2g.h03                .493908E-03
```

Case 3a

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead-lag-guard columns
Case 3a - SRS avg simulant, 5gpm ---> 2gpm at 500BVs, 35C, large particle size
1, 150, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNF                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
790.77, 48.68, 18927, 0.0d+0     Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.50, 0.24,  0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 1.4d-5, 1, 0.0           spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.022, 1.249                     fluid viscosity(poise), density(g/cm^3)
m                                COMMAND - subcolumns (carousel-concentration driven)
50, 150, 0, 1, 1.4d-8, 0.0, 150000   Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
s                                COMMAND - flow rate step change
12960, 7571, 1, 0                time(min), flow(ml/min), freq, dt(min)
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile (Col #1 Breakthrough)
-1,  3189, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #2 Breakthrough)
-1, 11546, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Col #3 Breakthrough)
-1, 57227, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
-                                end of commands
150000, 1                        end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
9.327d-5                         part-pore diffusivities(cm^2/min) 20% of free value
4.663d-4                         Brownian diffusivities(cm^2/min)
0.3395                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.861 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.5799 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
3.1236d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
 ==============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ==============================================================================
 Input file: Case3a
 TCCR Simulation of Cs removal on CST material lead-lag-guard columns
 Case 3a - SRS avg simulant, 5gpm ---> 2gpm at 500BVs, 35C, large particle s
 Begin Run:  16:33:03 on 11-29-2018   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6010
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 Sub-Column Boundary Conditions: Flux Continuity
 ==============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        = 150000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    790.77000 cm          D              =     48.68000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =1471774.26698 mL
 F              =  18927.00000 mL/min      Uo (linear)    =     20.33859 cm/min
 R              =    286.00000 microns     L/R            =  27649.30070
 Bed Void frac. =       .50000             Pcl. Porosity  =       .24000
 Spec. Area     =     52.44755 1/cm        Time/BV        =     12.96009 min
 Vol CSTRs      =       .00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
```

```
Eb  [cm2/min]  =  .27931E+01
Dp  [cm2/min]  =  .93270E-04
Doo [cm2/min]  =  .46630E-03
kf  [cm/min]   =  .19131E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .55040E+00
Sc(i)          =  .22664E+04
Peb(i)         =  .19194E+04
Bi(i)          =  .24443E+03
Nf(i)          =  .26007E+03
Np(i)          =  .35467E+00
Pep(i)         =  .25986E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .33950E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .31236E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1400E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2200E-01 poise and density to 1.249     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1500E+06 min.
     When comp.  1 reaches .1400E-07 M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Step change flow at .1296E+05 min to  .757E+04 mL/min
     Execute   1 times, every .0000     mins.
  5: Monitor conc. history at stream  2.  Filename = Case3a.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Monitor conc. history at stream  3.  Filename = Case3a.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  7: Monitor conc. history at stream  4.  Filename = Case3a.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  8: Dump full profile file at  3189.     min
     Execute   1 times, every .0000     mins.
  9: Dump full profile file at  .1155E+05 min
     Execute   1 times, every .0000     mins.
 10: Dump full profile file at  .5723E+05 min
     Execute   1 times, every .0000     mins.
===============================================================================
Conc. Carousel caused bed shift at t = .5726E+05 min
Conc. Carousel caused bed shift at t = .1085E+06 min
VERSE-LC finished in  7306 steps.  Average step size 20.53     minutes
End run:  16:41:15 on 11-29-2018
Integrated Areas in History Files:
Case3a.h01                 .507717
Case3a.h02                 .274963E-01
Case3a.h03                 .264642E-03
```

Case 5a

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead-lag columns
Case 5a_rev - Tank 10H Batch 1A, 5gpm, 34C, large particle size
1, 100, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNF                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
527.18, 48.68, 18927, 0.0d+0     Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.548, 0.24,  0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 1.131d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.0163, 1.1616                   fluid viscosity(poise), density(g/cm^3)
m                                COMMAND - subcolumns (carousel-concentration driven)
50, 100, 0, 1, 1.131d-8, 0.0, 1d+6   Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile (First Lag Col Breakthrough)
-1, 34960, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Second Lag Col Breakthrough)
-1, 65050, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Third Lag Col Breakthrough)
-1, 95940, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
-                                end of commands
150000, 1                        end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
1.9836d-4                        part-pore diffusivities(cm^2/min) 25% of free value
7.9343d-4                        Brownian diffusivities(cm^2/min) (calc. by OLI)
0.2662                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.9892 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.464 x 0.58 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
1.2358d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
==============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
==============================================================================
Input file: Case5a_rev
TCCR Simulation of Cs removal on CST material lead-lag columns
Case 5a_rev - Tank 10H Batch 1A, 5gpm, 34C, large particle size
Begin Run:  19:38:01 on 03-10-2019   running under Windows 95/8
Finite elements    - axial:100  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  4010
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? N   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
Sub-Column Boundary Conditions: Flux Continuity
==============================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        = 150000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    527.18000 cm          D              =     48.68000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      = 981182.84466 mL
F              =  18927.00000 mL/min      Uo (linear)    =     18.55710 cm/min
R              =    286.00000 microns     L/R            =  18432.86713
Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
Spec. Area     =     47.41259 1/cm        Time/BV        =     14.20426 min
Vol CSTRs      =       .00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .27804E+01
Dp  [cm2/min]  =  .19836E-03
Doo [cm2/min]  =  .79343E-03
kf  [cm/min]   =  .24878E+00
```

```
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .69088E+00
Sc(i)          =  .10611E+04
Peb(i)         =  .17593E+04
Bi(i)          =  .14946E+03
Nf(i)          =  .30574E+03
Np(i)          =  .82671E+00
Pep(i)         =  .11148E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .26620E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .12358E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units           M
==============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1131E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1630E-01 poise and density to 1.162     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .1131E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case5a_rev.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case5a_rev.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Dump full profile file at  .3496E+05 min
     Execute   1 times, every .0000     mins.
  7: Dump full profile file at  .6505E+05 min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  .9594E+05 min
     Execute   1 times, every .0000     mins.
==============================================================================
Conc. Carousel caused bed shift at t = .3506E+05 min
Conc. Carousel caused bed shift at t = .6523E+05 min
Conc. Carousel caused bed shift at t = .9620E+05 min
Conc. Carousel caused bed shift at t = .1271E+06 min
VERSE-LC finished in 12079 steps.  Average step size 12.42     minutes
End run:  19:44:02 on 03-10-2019
Integrated Areas in History Files:
Case5a_rev.h01             .800320E-01
Case5a_rev.h02             .187461E-03
```

Case 5b

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead-lag-guard columns
Case 5b_rev - Tank 10H Batch 1A, 3gpm, 34C, large particle size
1, 150, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNF                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
790.76, 48.68, 11356, 0.0d+0     Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.548, 0.24,  0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 1.131d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.0163, 1.1616                   fluid viscosity(poise), density(g/cm^3)
m                                COMMAND - subcolumns (carousel-concentration driven)
50, 150, 0, 1, 1.131d-8, 0.0, 1d+6   Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile (First Lag Col Breakthrough)
-1, 136600, 1, 0                 particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Second Lag Col Breakthrough)
-1, 202700, 1, 0                 particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Third Lag Col Breakthrough)
-1, 271840, 1, 0                 particle point (-1 for all), time(min), freq, dt(min)
-                                end of commands
300000, 1                        end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
1.9836d-4                        part-pore diffusivities(cm^2/min) 25% of free value
7.9343d-4                        Brownian diffusivities(cm^2/min) (calc. by OLI)
0.2662                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=1.0175 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.45 x 0.58 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
1.2358d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: Case5b_rev
 TCCR Simulation of Cs removal on CST material lead-lag-guard columns
 Case 5b_rev - Tank 10H Batch 1A, 3gpm, 34C, large particle size
 Begin Run:  19:44:16 on 03-10-2019   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6010
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 Sub-Column Boundary Conditions: Flux Continuity
 ===============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        = 300000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    790.76000 cm          D              =     48.68000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =1471755.65507 mL
 F              =  11356.00000 mL/min      Uo (linear)    =     11.13407 cm/min
 R              =    286.00000 microns     L/R            =  27648.95105
 Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
 Spec. Area     =     47.41259 1/cm        Time/BV        =     23.67389 min
 Vol CSTRs      =       .00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .16843E+01
 Dp  [cm2/min]  =  .19836E-03
```

```
Doo [cm2/min]  =  .79343E-03
kf  [cm/min]   =  .20983E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .41452E+00
Sc(i)          =  .10611E+04
Peb(i)         =  .17424E+04
Bi(i)          =  .12606E+03
Nf(i)          =  .42978E+03
Np(i)          =  .13779E+01
Pep(i)         =  .66889E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .26620E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .12358E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1131E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1630E-01 poise and density to 1.162     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .1131E-07 M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case5b_rev.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case5b_rev.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = Case5b_rev.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  7: Dump full profile file at  .1366E+06 min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  .2027E+06 min
     Execute   1 times, every .0000     mins.
  9: Dump full profile file at  .2718E+06 min
     Execute   1 times, every .0000     mins.
===============================================================================
Conc. Carousel caused bed shift at t = .1370E+06 min
Conc. Carousel caused bed shift at t = .2032E+06 min
Conc. Carousel caused bed shift at t = .2726E+06 min
VERSE-LC finished in 12691 steps.  Average step size 23.64     minutes
End run:  19:46:07 on 03-10-2019
Integrated Areas in History Files:
Case5b_rev.h01            1.31580
Case5b_rev.h02             .737170E-01
Case5b_rev.h03             .313581E-03
```

Case 5c

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead-lag columns
Case 5c_rev - Tank 10H Batch 1A, 5gpm, 34C, large particle size
1, 100, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNF                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
527.18, 48.68, 18927, 0.0d+0     Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.548, 0.24,  0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 1.131d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.0163, 1.1616                   fluid viscosity(poise), density(g/cm^3)
m                                COMMAND - subcolumns (carousel-concentration driven)
50, 100, 0, 1, 1.131d-8, 0.0, 1d+6   Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile (First Lag Col Breakthrough)
-1, 19400, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Second Lag Col Breakthrough)
-1, 36125, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                COMMAND - dump column profile (Third Lag Col Breakthrough)
-1, 53280, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
-                                end of commands
150000, 1                        end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
1.9836d-4                        part-pore diffusivities(cm^2/min) 25% of free value
7.9343d-4                        Brownian diffusivities(cm^2/min) (calc. by OLI)
0.144                            Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.9892 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.251 x 0.58 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
1.2358d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
==============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
==============================================================================
Input file: Case5c_rev
TCCR Simulation of Cs removal on CST material lead-lag columns
Case 5c_rev - Tank 10H Batch 1A, 5gpm, 34C, large particle size
Begin Run:  20:05:44 on 03-10-2019   running under Windows 95/8
Finite elements    - axial:100  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  4010
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? N   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
Sub-Column Boundary Conditions: Flux Continuity
==============================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        = 150000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    527.18000 cm          D              =     48.68000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      = 981182.84466 mL
F              =  18927.00000 mL/min      Uo (linear)    =     18.55710 cm/min
R              =    286.00000 microns     L/R            =  18432.86713
Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
Spec. Area     =     47.41259 1/cm        Time/BV        =     14.20426 min
Vol CSTRs      =       .00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .27804E+01
Dp  [cm2/min]  =  .19836E-03
Doo [cm2/min]  =  .79343E-03
kf  [cm/min]   =  .24878E+00
```

```
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .69088E+00
Sc(i)          =  .10611E+04
Peb(i)         =  .17593E+04
Bi(i)          =  .14946E+03
Nf(i)          =  .30574E+03
Np(i)          =  .82671E+00
Pep(i)         =  .11148E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .14400E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .12358E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
==============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1131E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1630E-01 poise and density to 1.162     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .1131E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case5c_rev.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case5c_rev.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Dump full profile file at  .1940E+05 min
     Execute   1 times, every .0000     mins.
  7: Dump full profile file at  .3613E+05 min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  .5328E+05 min
     Execute   1 times, every .0000     mins.
==============================================================================
Conc. Carousel caused bed shift at t = .1901E+05 min
Conc. Carousel caused bed shift at t = .3534E+05 min
Conc. Carousel caused bed shift at t = .5210E+05 min
Conc. Carousel caused bed shift at t = .6885E+05 min
Conc. Carousel caused bed shift at t = .8559E+05 min
Conc. Carousel caused bed shift at t = .1023E+06 min
Conc. Carousel caused bed shift at t = .1191E+06 min
Conc. Carousel caused bed shift at t = .1358E+06 min
VERSE-LC finished in 10778 steps.  Average step size 13.92     minutes
End run:  20:07:17 on 03-10-2019
Integrated Areas in History Files:
Case5c_rev.h01            .835915E-01
Case5c_rev.h02            .211572E-03
```

Case 5d

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead-lag-guard columns
Case 5d_rev - Tank 10H Batch 1A, 3gpm, 34C, large particle size
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNF                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                 comp-conc units
790.76, 48.68, 11356, 0.0d+0      Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.548, 0.24,  0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentrations (M)
S                                 COMMAND - inlet conc step change
1, 0.0, 1.131d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.0163, 1.1616                    fluid viscosity(poise), density(g/cm^3)
m                                 COMMAND - subcolumns (carousel-concentration driven)
50, 150, 0, 1, 1.131d-8, 0.0, 1d+6   Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                 COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5            unit op#, ptscale(1-4) filtering
D                                 COMMAND - dump column profile (First Lag Col Breakthrough)
-1, 75880, 1, 0                   particle point (-1 for all), time(min), freq, dt(min)
D                                 COMMAND - dump column profile (Second Lag Col Breakthrough)
-1, 112610, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
D                                 COMMAND - dump column profile (Third Lag Col Breakthrough)
-1, 151030, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
-                                 end of commands
300000, 1                         end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                    abs-tol, rel-tol
-                                 non-negative conc constraint
1.0d0                             size exclusion factor
1.9836d-4                         part-pore diffusivities(cm^2/min) 25% of free value
7.9343d-4                         Brownian diffusivities(cm^2/min) (calc. by OLI)
0.144                             Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.9892 g/ml
1.0                               Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                               Freundlich/Langmuir Hybrid Ma   (-)            a = 0.25 x 0.58 x rhob
1.0                               Freundlich/Langmuir Hybrid Mb   (-)
1.2358d-4                         Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: Case5d_rev
 TCCR Simulation of Cs removal on CST material lead-lag-guard columns
 Case 5d_rev - Tank 10H Batch 1A, 3gpm, 34C, large particle size
 Begin Run:  20:07:54 on 03-10-2019   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6010
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 Sub-Column Boundary Conditions: Flux Continuity
 ===============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        = 300000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    790.76000 cm          D              =     48.68000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =1471755.65507 mL
 F              =  11356.00000 mL/min      Uo (linear)    =     11.13407 cm/min
 R              =    286.00000 microns     L/R            =  27648.95105
 Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
 Spec. Area     =     47.41259 1/cm        Time/BV        =     23.67389 min
 Vol CSTRs      =       .00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .16843E+01
 Dp  [cm2/min]  =  .19836E-03
```

```
Doo [cm2/min]  =  .79343E-03
kf  [cm/min]   =  .20983E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .41452E+00
Sc(i)          =  .10611E+04
Peb(i)         =  .17424E+04
Bi(i)          =  .12606E+03
Nf(i)          =  .42978E+03
Np(i)          =  .13779E+01
Pep(i)         =  .66889E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .14400E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .12358E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1131E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1630E-01 poise and density to 1.162     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .1131E-07 M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case5d_rev.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case5d_rev.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = Case5d_rev.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  7: Dump full profile file at  .7588E+05 min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  .1126E+06 min
     Execute   1 times, every .0000     mins.
  9: Dump full profile file at  .1510E+06 min
     Execute   1 times, every .0000     mins.
===============================================================================
Conc. Carousel caused bed shift at t = .7413E+05 min
Conc. Carousel caused bed shift at t = .1100E+06 min
Conc. Carousel caused bed shift at t = .1475E+06 min
Conc. Carousel caused bed shift at t = .1862E+06 min
Conc. Carousel caused bed shift at t = .2258E+06 min
Conc. Carousel caused bed shift at t = .2662E+06 min
VERSE-LC finished in 12700 steps.  Average step size 23.62     minutes
End run:  20:09:40 on 03-10-2019
Integrated Areas in History Files:
Case5d_rev.h01            1.11901
Case5d_rev.h02            .616759E-01
Case5d_rev.h03            .403477E-03
```

Case 5e

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead-lag columns
Case 5e_rev - Tank 10H Batch 1A, 5gpm, 34C, large particle size
1, 100, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNF                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                 comp-conc units
527.18, 48.68, 18927, 0.0d+0      Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.548, 0.24,  0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentrations (M)
S                                 COMMAND - inlet conc step change
1, 0.0, 1.131d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.0163, 1.1616                    fluid viscosity(poise), density(g/cm^3)
m                                 COMMAND - subcolumns (carousel-concentration driven)
50, 100, 0, 1, 1.131d-8, 0.0, 1d+6   Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                 COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5            unit op#, ptscale(1-4) filtering
D                                 COMMAND - dump column profile (First Lag Col Breakthrough)
-1, 52805, 1, 0                   particle point (-1 for all), time(min), freq, dt(min)
D                                 COMMAND - dump column profile (Second Lag Col Breakthrough)
-1, 98260, 1, 0                   particle point (-1 for all), time(min), freq, dt(min)
D                                 COMMAND - dump column profile (Third Lag Col Breakthrough)
-1, 144930, 1, 0                  particle point (-1 for all), time(min), freq, dt(min)
-                                 end of commands
150000, 1                         end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                    abs-tol, rel-tol
-                                 non-negative conc constraint
1.0d0                             size exclusion factor
1.9836d-4                         part-pore diffusivities(cm^2/min) 25% of free value
7.9343d-4                         Brownian diffusivities(cm^2/min) (calc. by OLI)
0.3901                            Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.9892 g/ml
1.0                               Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                               Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.58 x rhob
1.0                               Freundlich/Langmuir Hybrid Mb   (-)
1.2358d-4                         Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
=============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
=============================================================================
Input file: Case5e_rev
TCCR Simulation of Cs removal on CST material lead-lag columns
Case 5e_rev - Tank 10H Batch 1A, 5gpm, 34C, large particle size
Begin Run:  21:28:19 on 03-10-2019   running under Windows 95/8
Finite elements    - axial:100  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  4010
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? N   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
Sub-Column Boundary Conditions: Flux Continuity
=============================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        = 150000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    527.18000 cm          D              =     48.68000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      = 981182.84466 mL
F              =  18927.00000 mL/min      Uo (linear)    =     18.55710 cm/min
R              =    286.00000 microns     L/R            =  18432.86713
Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
Spec. Area     =     47.41259 1/cm        Time/BV        =     14.20426 min
Vol CSTRs      =       .00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .27804E+01
Dp  [cm2/min]  =  .19836E-03
Doo [cm2/min]  =  .79343E-03
kf  [cm/min]   =  .24878E+00
```

```
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .69088E+00
Sc(i)          =  .10611E+04
Peb(i)         =  .17593E+04
Bi(i)          =  .14946E+03
Nf(i)          =  .30574E+03
Np(i)          =  .82671E+00
Pep(i)         =  .11148E+05

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .39010E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .12358E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1131E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1630E-01 poise and density to 1.162     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .1131E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case5e_rev.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case5e_rev.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Dump full profile file at  .5281E+05 min
     Execute   1 times, every .0000     mins.
  7: Dump full profile file at  .9826E+05 min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  .1449E+06 min
     Execute   1 times, every .0000     mins.
===============================================================================
Conc. Carousel caused bed shift at t = .5137E+05 min
Conc. Carousel caused bed shift at t = .9556E+05 min
Conc. Carousel caused bed shift at t = .1409E+06 min
VERSE-LC finished in 12410 steps.  Average step size 12.09     minutes
End run:  21:36:20 on 03-10-2019
Integrated Areas in History Files:
Case5e_rev.h01             .840471E-01
Case5e_rev.h02             .194691E-03
```

Case 5f

VERSE Input:

```
TCCR Simulation of Cs removal on CST material lead-lag-guard columns
Case 5f_rev - Tank 10H Batch 1A, 3gpm, 34C, large particle size
1, 150, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNF                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,use datafile.yio,generate/update datafile.yio
M                                comp-conc units
790.76, 48.68, 11356, 0.0d+0     Total bed length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.0, 0.548, 0.24,  0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - inlet conc step change
1, 0.0, 1.131d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.0163, 1.1616                   fluid viscosity(poise), density(g/cm^3)
m                                COMMAND - subcolumns (carousel-concentration driven)
50, 150, 0, 1, 1.131d-8, 0.0, 1d+6   Nelem shift, Nelem watch, Npp watch, Nc watch, Cthresh, te, tee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
3, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D                                COMMAND - dump column profile (First Lag Col Breakthrough)
-1, 206360, 1, 0                 particle point (-1 for all), time(min), freq, dt(min)
-                                end of commands
300000, 1                        end time(min), max step size (B.V.)
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
1.9836d-4                        part-pore diffusivities(cm^2/min) 25% of free value
7.9343d-4                        Brownian diffusivities(cm^2/min) (calc. by OLI)
0.3901                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.9892 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)          Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)            a = 0.68 x 0.58 x rhob
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
1.2358d-4                        Freundlich/Langmuir Hybrid beta (-)
```

VERSE Output

```
==============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
==============================================================================
Input file: Case5f_rev
TCCR Simulation of Cs removal on CST material lead-lag-guard columns
Case 5f_rev - Tank 10H Batch 1A, 3gpm, 34C, large particle size
Begin Run:  08:39:40 on 03-12-2019   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6010
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? N   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
Sub-Column Boundary Conditions: Flux Continuity
==============================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        = 300000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    790.76000 cm          D              =     48.68000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =1471755.65507 mL
F              =  11356.00000 mL/min      Uo (linear)    =     11.13407 cm/min
R              =    286.00000 microns     L/R            =  27648.95105
Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
Spec. Area     =     47.41259 1/cm        Time/BV        =     23.67389 min
Vol CSTRs      =       .00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .16843E+01
Dp  [cm2/min]  =  .19836E-03
Doo [cm2/min]  =  .79343E-03
kf  [cm/min]   =  .20983E+00
Ds  [cm2/min]  =  .00000E+00
```

```
Dimensionless Groups:
Re             =  .41452E+00
Sc(i)          =  .10611E+04
Peb(i)         =  .17424E+04
Bi(i)          =  .12606E+03
Nf(i)          =  .42978E+03
Np(i)          =  .13779E+01
Pep(i)         =  .66889E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .39010E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .12358E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
==============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .1131E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1630E-01 poise and density to 1.162     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .1131E-07 M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = Case5f_rev.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  3.  Filename = Case5f_rev.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = Case5f_rev.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  7: Dump full profile file at  .2064E+06 min
     Execute   1 times, every .0000     mins.
==============================================================================
Conc. Carousel caused bed shift at t = .2007E+06 min
Conc. Carousel caused bed shift at t = .2978E+06 min
VERSE-LC finished in 12695 steps.  Average step size 23.63     minutes
End run:  08:50:36 on 03-12-2019
Integrated Areas in History Files:
Case5f_rev.h01             1.43770
Case5f_rev.h02             .823106E-01
Case5f_rev.h03             .290078E-03
```

Distribution:
timothy.brown@srnl.doe.gov
alex.cozzi@srnl.doe.gov
david.crowley@srnl.doe.gov
c.diprete@srnl.doe.gov
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samuel.fink@srnl.doe.gov
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Records Administration (EDWS)